Communications in Combinatorics and Optimization
Vol. 7, No. 2 (2022), pp.275-300
DOI: 10.22049/CCO.2021.27254.1221

CCO
Commun. Comb. Optim.

Research Article

Terminal status of vertices and terminal status connectivity indices of graphs with its applications to properties of cycloalkanes

Harishchandra S. Ramane[*†], **Kavita Bhajantri**[‡], **Deepa V. Kitturmath**[§]

Department of Mathematics, Karnatak University, Dharwad - 580003, India
[†]hsramane@yahoo.com
[‡]kavitabhajantri5@gmail.com
[§]deepakitturmath@gmail.com

Received: 12 May 2021; Accepted: 9 August 2021
Published Online: 11 August 2021

Abstract: In this article the terminal status of a vertex and terminal status connectivity indices of a connected graph have introduced. Explicit formulae for the terminal status of vertices and for terminal status connectivity indices of certain graphs are obtained. Also some bounds are given for these indices. Further these indices are used for predicting the physico-chemical properties of cycloalkanes and it is observed that the correlation of physico-chemical properties of cycloalkanes with newly introduced indices is better than the correlation with other indices.

Keywords: Terminal status of a vertex, terminal status connectivity indices, pendent vertex, diameter of a graph, molecular graph

AMS Subject classification: 05C12

1. Introduction

The topological index, a graph invariant, is the numerical quantity associated with the graph structure. It can be utilized for modeling the information such as quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) of molecules in theoretical chemistry. Several such indices based on the degrees and distances in a graph have been proposed and studied [9–11, 21]. In this paper we define the terminal status of a vertex and hence define the terminal status connectivity indices of a connected graph based on the distance. Further we

* *Corresponding Author*

give explicit formulae for the terminal status of a vertex and for terminal status indices of some graphs. Also obtain bounds for these indices and carry regression analysis of terminal status connectivity indices with the physico-chemical properties of cycloalkanes.

Let G be a simple, connected graph with n vertices and m edges. Let its vertex set be $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. The edge joining the vertices u and v is denoted by uv. Two vertices are said to be *neighbors* of each other if they are adjacent. The *degree* of a vertex u in a graph G is the number of its neighbors and is denoted by $d_G(u)$. A vertex u is said to be *terminal vertex* or *pendent vertex* if $d_G(u) = 1$. In G, the *distance* between the vertices u and v is the length of the shortest path joining them and is denoted by $d_G(u, v)$. The *diameter* of a graph G, denoted by $diam(G)$ is the maximum distance between any pair of vertices of G. The *status* of a vertex u, denoted by $\sigma_G(u)$ is defined as

$$\sigma_G(u) = \sum_{v \in V(G)} d_G(u, v). \tag{1}$$

The *Wiener index* of a graph G, denoted by $W(G)$, is defined as the sum of the distances between all pairs of vertices of G. That is

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v) = \frac{1}{2} \sum_{u \in V(G)} \sigma_G(u).$$

This molecular structure descriptor was introduced by Wiener [35] in 1947. For details on its chemical applications and mathematical properties one may refer to [3, 4, 14, 20, 29, 33, 34].

If the graph G has k pendent vertices $v_1, v_2, \ldots, v_k$, then its *terminal distance matrix* is the square matrix of order k whose (i, j)-th entry is $d_G(v_i, v_j)$. Terminal distance matrices were used for modeling amino acid sequences of proteins and of the genetic codes [17, 27, 28].

The *terminal Wiener index* $TW(G)$ of a connected graph G is defined as the sum of the distances between all pairs of its pendent vertices.
Thus, if $V_T(G) = \{v_1, v_2, \ldots, v_k\}$ is the set of all pendent vertices of G, then

$$TW(G) = \sum_{1 \leq i < j \leq k} d_G(v_i, v_j).$$

This distance-based molecular structure descriptor was put forward by Gutman, Furtula and Petrović [12]. The same was also studied by Székely, Wang and Wu [30].

More on the terminal Wiener index can be found in [2, 8, 16, 23].

Analogous to the Eq. (1), we define here the *terminal status* of a vertex u as

$$ts_G(u) = \sum_{v \in V_T(G)} d_G(u,v),$$

where $V_T(G)$ is the set of all pendent vertices of G. Therefore

$$TW(G) = \frac{1}{2} \sum_{u \in V_T(G)} ts_G(u).$$

The first and second *Zagreb indices* of a graph G are defined as [15]

$$M_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)] \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v).$$

The Zagreb indices were used in the structure property model [13, 18, 19, 22, 31]. The first and second *status connectivity indices* of a connected graph G are defined as [24, 25]

$$S_1(G) = \sum_{uv \in E(G)} [\sigma_G(u) + \sigma_G(v)] \quad \text{and} \quad S_2(G) = \sum_{uv \in E(G)} \sigma_G(u)\sigma_G(v).$$

There are several other indices such as eccentricity index [1, 32], Randic index [6, 26], degree distance of a graph [5, 7] etc.

Motivated by the invariants as above, we define here *first terminal status connectivity index* $TS_1(G)$ and *second terminal status connectivity index* $TS_2(G)$ of a connected graph G as:

$$TS_1(G) = \sum_{uv \in E(G)} [ts_G(u) + ts_G(v)] \tag{2}$$

and

$$TS_2(G) = \sum_{uv \in E(G)} ts_G(u) ts_G(v). \tag{3}$$

The Eq. (2) can be expressed as

$$TS_1(G) = \sum_{u \in V(G)} d_G(u) ts_G(u).$$

The vertex set of a graph given in Fig. 1 is $V(G) = \{v_1, v_2, v_3, v_4, v_5, v_6, v_7\}$ and pendent vertex set is $V_T(G) = \{v_1, v_2, v_7\}$. The terminal status of vertices of G are

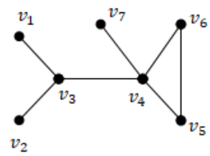

Figure 1. **Graph** G

$ts_G(v_1) = 5$, $ts_G(v_2) = 5$, $ts_G(v_3) = 4$, $ts_G(v_4) = 5$, $ts_G(v_5) = 8$, $ts_G(v_6) = 8$ and $ts_G(v_7) = 6$. Therefore $TS_1(G) = 80$ and $TS_2(G) = 234$.

In Section 2 we obtain the terminal status of vertices and in Section 3 we obtain the terminal status connectivity indices. In Section 4 we carry the regression analysis of indices and physico-chemical properties of cycloalkanes followed by the Section 5 as conclusion.

2. Terminal status of vertices

In this section we find terminal status of the vertices of a graph.

Observations

1. If G has no pendent vertex then $ts_G(u) = 0$ for all $u \in V(G)$.
2. If G has exactly one pendent vertex, say u, then $ts_G(u) = 0$.
3. If G has at least one pendent vertex, then $ts_G(u) \geq 1$, where u is not a pendent vertex.
4. If G has at least two pendent vertices, then $ts_G(u) \geq 1$ for all $u \in V(G)$.
5. There is no pendent vertex in G such that $ts_G(u) = 1$, except for $G \cong K_2$, where K_n is a complete graph on n vertices.

Theorem 1. *Let G be a connected graph with n vertices and $diam(G) \leq 2$. Let u be the vertex having pendent neighbor. Then $d_G(u) = n - 1$.*

Proof. For any vertex u, $d_G(u) \leq n - 1$. Let u be the vertex having pendent neighbor. Suppose $d_G(u) < n - 1$, then there exists a vertex, say v, which is not adjacent to u. Then the distance between vertex v and any pendent vertex is greater than 2. This contradicts to the fact that $diam(G) \leq 2$. Hence $d_G(u) = n - 1$. □

Theorem 2. *Let G be a connected graph with n vertices and $diam(G) = 2$. Then there exists a unique vertex having pendent neighbor.*

Proof. Suppose there are two vertices say u and v having pendent neighbors. Without loss of generality, let u' be the pendent neighbor of u and v' be the pendent neighbor of v. Then $d_G(u', v') > 2$. This contradicts to the fact that $diam(G) = 2$. Hence the result follows. □

Theorem 3. *Let G be a graph on n vertices with $diam(G) \leq 2$ and n_t be the number of pendent vertices of G.*
(i) *If u is not a pendent vertex, then*

$$ts_G(u) = \begin{cases} 2n_t, & \text{if } u \text{ has no pendent neighbor} \\ n_t, & \text{if } u \text{ has pendent neighbor.} \end{cases}$$

(ii) *If u is a pendent vertex, then*

$$ts_G(u) = \begin{cases} 1, & \text{for } n = 2 \\ 2(n_t - 1), & \text{for } n \geq 3. \end{cases}$$

Proof. (i) Let u be a non pendent vertex having no pendent neighbor. Then the distance between vertex u and any pendent vertex is 2. There are n_t pendent vertices in G. Therefore $ts_G(u) = 2n_t$.
Similarly if u is non pendent vertex having pendent neighbor, then the distance between vertex u and any pendent vertex is 1. There are n_t pendent vertices in G. Therefore $ts_G(u) = n_t$.

(ii) If $n = 2$, then $G \cong K_2$. Hence for any pendent vertex u of K_2, $ts_G(u) = 1$. Now let $n \geq 3$ and let u be the pendent vertex in G. Then distance between u and other pendent vertex is 2. There are $n_t - 1$ pendent vertices other than u in G. Therefore $ts_G(u) = 2(n_t - 1)$. □

The following is a consequence of Theorem 3.

Corollary 1. *Let $K_{1,n-1}$ be a star on $n \geq 3$ vertices. Then*

$$ts_{K_{1,n-1}}(u) = \begin{cases} n - 1, & \text{if } u \text{ is a central vertex of } K_{1,n-1} \\ 2(n-2), & \text{if } u \text{ is a pendent vertex of } K_{1,n-1}. \end{cases}$$

Theorem 4. *Let P_n be a path on n vertices. Then $ts_{P_n}(u) = n - 1$ for all $u \in V(P_n)$.*

Proof. Let $u_1, u_2, \ldots, u_n$ be the vertices of a path P_n such that u_i is adjacent to u_{i+1}, $i = 1, 2, \ldots, n-1$. Hence u_1 and u_n are the pendent vertices of P_n. Therefore for $i = 1, 2, \ldots, n$

$$\begin{aligned} ts_{P_n}(u_i) &= d_{P_n}(u_i, u_1) + d_{P_n}(u_i, u_n) \\ &= (i-1) + (n-i) \\ &= n-1. \end{aligned}$$

□

The graph G^{+k} is obtained from G by attaching k pendent vertices to each vertex of G (see Fig. 2).

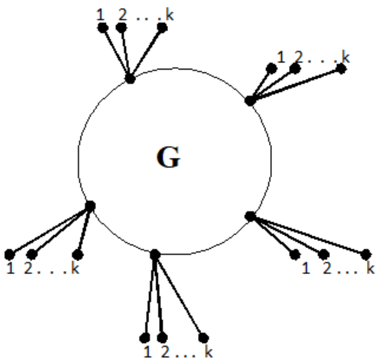

Figure 2. **Graph G^{+k}.**

Theorem 5. *Let G be a connected graph on n vertices with vertex set $V(G)$. Then for $k \geq 1$,*

$$ts_{G^{+k}}(u) = \begin{cases} 2nk - 2 + k\sigma_G(v), & \text{if } u \text{ is a pendent vertex in } G^{+k} \text{ adjacent to } v \in V(G) \\ nk + k\sigma_G(u), & \text{if } u \text{ is not a pendent vertex in } G^{+k}. \end{cases}$$

Proof. Without loss of generality, let the vertices of G be $v_1, v_2, \ldots, v_n$. We consider two cases.

Case 1. Let u be the pendent vertex in G^{+k} adjacent to $v_1 = v \in V(G)$. Then the sum of distances between vertex u and the $(k-1)$ pendent vertices adjacent to v_1 is $2(k-1)$. The sum of distances from u to k pendent vertices adjacent to

$v_i \in V(G) \setminus \{v_1\}$ is $k(2 + d_G(v, v_i))$, $i = 2, 3, \ldots, n$. Therefore

$$\begin{aligned} ts_{G^{+k}}(u) &= 2(k-1) + \sum_{i=2}^{n} k(2 + d_G(v_1, v_i)) \\ &= 2(k-1) + 2k(n-1) + k\sum_{i=2}^{n} d_G(v_1, v_i) \\ &= 2nk - 2 + k\sigma_G(v_1) \\ &= 2nk - 2 + k\sigma_G(v). \end{aligned}$$

Case 2. Let u be the non pendent vertex in G^{+k}. Without loss of generality, let $u = v_1$. Then the sum of distances between vertex u and pendent vertices adjacent to u is k. The sum of distances from $u = v_1$ to k pendent vertices adjacent to $v_i \in V(G) \setminus \{v_1\}$ is $k + kd_G(v_1, v_i)$, $i = 2, 3, \ldots, n$. Therefore

$$\begin{aligned} ts_{G^{+k}}(u) &= k + \sum_{i=2}^{n} [k + kd_G(v_1, v_i)] \\ &= k + k(n-1) + k\sum_{i=2}^{n} d_G(v_1, v_i) \\ &= nk + k\sigma_G(v_1) \\ &= nk + k\sigma_G(u). \end{aligned}$$

□

Theorem 6. *Let G be a graph on $n \geq 3$ vertices with $diam(G) = D$ and n_t be the number of pendent vertices of G.*
(i) If u is not a pendent vertex and has no pendent neighbor, then

$$2n_t \leq ts_G(u) \leq Dn_t.$$

(ii) If u is not a pendent vertex and has n_u number of pendent neighbors, then

$$2n_t - n_u \leq ts_G(u) \leq n_u + (D-1)(n_t - n_u).$$

(iii) If u is a pendent vertex, then

$$2(n_t - 1) \leq ts_G(u) \leq D(n_t - 1).$$

Proof. (i) Let u be a non pendent vertex having no pendent neighbor. Then the distance between vertex u and any pendent vertex is at least 2 and at most D. There are n_t pendent vertices in G. Therefore $2n_t \leq ts_G(u) \leq Dn_t$.

(ii) Let u be a non pendent vertex having n_u number of pendent neighbors. Then the distance between vertex u and these n_u pendent vertices is 1 and the distance between u and remaining $n_t - n_u$ pendent vertices is at least 2 and at most $D-1$. Therefore $n_u + 2(n_t - n_u) = 2n_t - n_u \leq ts_G(u) \leq n_u + (D-1)(n_t - n_u)$.

(iii) Let u be the pendent vertex in G. Then distance between u and other pendent vertex is at least 2 and at most D. There are $n_t - 1$ pendent vertices other than u in G. Therefore $2(n_t - 1) \leq ts_G(u) \leq D(n_t - 1)$. □

3. Terminal status connectivity indices of graphs

In this section we obtain the terminal status connectivity indices of graphs. Also we give the bounds for these indices.

Observations

1. If G has no pendent vertex then $TS_1(G) = 0$ and $TS_2(G) = 0$.
2. If G has at least one pendent vertex, then $TS_1(G) \geq 2$ and $TS_2(G) \geq 1$.
3. By the definitions of status connectivity indices and terminal status connectivity indices, we have $S_1(G) \geq TS_1(G)$ and $S_2(G) \geq TS_2(G)$.

Theorem 7. *Let G be a connected graph with $diam(G) = 2$ having n vertices, m edges and n_t pendent vertices. Then*

$$TS_1(G) = n_t(4m - n - 1)$$

and

$$TS_2(G) = 2n_t^2(2m - n).$$

Proof. Here $n \geq 3$ as $diam(G) = 2$. The edge set $E(G)$ of a graph G can be partitioned into three sets E_1, E_2 and E_3, where
$E_1 = \{uv \mid u$ and v has no pendent neighbor. Further $d_G(u) > 1$ and $d_G(v) > 1\}$,
$E_2 = \{uv \mid u$ has pendent neighbor but v does not or vice-versa and $d_G(u), d_G(v) > 1\}$ and
$E_3 = \{uv \mid$ either u or v is a pendent vertex$\}$.
It is easy to check that $|E_1| = m - n + 1$, $|E_2| = n - n_t - 1$ and $|E_3| = n_t$.
Further by Theorem 3, we have, if u is not a pendent vertex, then

$$ts_G(u) = \begin{cases} 2n_t, & \text{if } u \text{ has no pendent neighbor} \\ n_t, & \text{if } u \text{ has pendent neighbor} \end{cases}$$

and if u is a pendent vertex, then $ts_G(u) = 2(n_t - 1)$.
Therefore

$$\begin{aligned}
TS_1(G) &= \sum_{uv \in E(G)} [ts_G(u) + ts_G(v)] \\
&= \sum_{uv \in E_1} [ts_G(u) + ts_G(v)] + \sum_{uv \in E_2} [ts_G(u) + ts_G(v)] + \sum_{uv \in E_3} [ts_G(u) + ts_G(v)] \\
&= \sum_{uv \in E_1} [2n_t + 2n_t] + \sum_{uv \in E_2} [n_t + 2n_t] + \sum_{uv \in E_3} [2(n_t - 1) + n_t] \\
&= 4n_t(m - n + 1) + 3n_t(n - n_t - 1) + n_t(3n_t - 2) \\
&= n_t(4m - n - 1)
\end{aligned}$$

and

$$\begin{aligned}
TS_2(G) &= \sum_{uv \in E(G)} ts_G(u) ts_G(v) \\
&= \sum_{uv \in E_1} ts_G(u) ts_G(v) + \sum_{uv \in E_2} ts_G(u) ts_G(v) + \sum_{uv \in E_3} ts_G(u) ts_G(v) \\
&= \sum_{uv \in E_1} (2n_t)(2n_t) + \sum_{uv \in E_2} (n_t)(2n_t) + \sum_{uv \in E_3} (2(n_t - 1))(n_t) \\
&= 4n_t^2(m - n + 1) + 2n_t^2(n - nt - 1) + 2n_t^2(n_t - 1) \\
&= 2n_t^2(2m - n).
\end{aligned}$$

□

Corollary 2. *Let $K_{1,n-1}$ be a star on $n \geq 3$ vertices. Then*

$$TS_1(K_{1,n-1}) = (n-1)(3n-5)$$

and

$$TS_2(K_{1,n-1}) = 2(n-1)^2(n-2).$$

Theorem 8. *Let P_n be a path on n vertices. Then*

$$TS_1(P_n) = 2(n-1)^2$$

and

$$TS_2(P_n) = (n-1)^3.$$

Proof. By Theorem 4, we have, $ts_{P_n}(u) = n-1$ for all $u \in V(P_n)$. Therefore

$$\begin{aligned} TS_1(P_n) &= \sum_{uv \in E(P_n)} [ts_{P_n}(u) + ts_{P_n}(v)] \\ &= \sum_{uv \in E(P_n)} 2(n-1) \\ &= 2(n-1)^2 \end{aligned}$$

and

$$\begin{aligned} TS_2(P_n) &= \sum_{uv \in E(P_n)} ts_{P_n}(u) ts_{P_n}(v) \\ &= \sum_{uv \in E(P_n)} (n-1)^2 \\ &= (n-1)^3. \end{aligned}$$

□

Theorem 9. *Let G be a graph with n vertices and m edges. Then for $k \geq 1$*

$$TS_1(G^{+k}) = nk(3nk-2) + 2mnk + kS_1(G) + 4k^2W(G)$$

and

$$\begin{aligned} TS_2(G^{+k}) &= 2n^2k^2(nk-1) + 2k^2(3nk-2)W(G) + k^3 \sum_{v \in V(G)} (\sigma_G(u))^2 \\ &\quad + mn^2k^2 + nk^2S_1(G) + k^2S_2(G). \end{aligned}$$

Proof. By Theorem 5

$$ts_{G^{+k}}(u) = \begin{cases} 2nk - 2 + k\sigma_G(v), & \text{if } u \text{ is a pendent vertex in } G^{+k} \text{ adjacent to } v \in V(G) \\ nk + k\sigma_G(u), & \text{if } u \text{ is non pendent vertex.} \end{cases}$$

The edge set $E(G^{+k})$ can be partitioned into two sets E_1 and E_2, where
$E_1 = \{uv \mid u \text{ is a pendent vertex and } v \text{ is non pendent vertex}\}$ and
$E_2 = \{uv \mid u \text{ and } v \text{ are non pendent vertices}\}$. It is easy to check that $|E_1| = nk$ and

$|E_2| = m$. Therefore

$$\begin{aligned}
TS_1(G^{+k}) &= \sum_{uv\in E(G^{+k})} (ts_{G^{+k}}(u) + ts_{G^{+k}}(v)) \\
&= \sum_{uv\in E_1} (ts_{G^{+k}}(u) + ts_{G^{+k}}(v)) + \sum_{uv\in E_2} (ts_{G^{+k}}(u) + ts_{G^{+k}}(v)) \\
&= \sum_{uv\in E_1} (2nk - 2 + k\sigma_G(v) + nk + k\sigma_G(v)) \\
&\quad + \sum_{uv\in E_2} (nk + k\sigma_G(u) + nk + k\sigma_G(v)) \\
&= \sum_{uv\in E_1} (3nk - 2 + 2k\sigma_G(v)) + \sum_{uv\in E_2} (2nk + k(\sigma_G(u) + \sigma_G(v))) \\
&= nk(3nk-2) + 2k^2 \sum_{v\in V(G)} \sigma_G(v) + 2mnk + k \sum_{uv\in E(G)} (\sigma_G(u) + \sigma_G(v)) \\
&= nk(3nk-2) + 2mnk + 4k^2 W(G) + kS_1(G)
\end{aligned}$$

and

$$\begin{aligned}
TS_2(G^{+k}) &= \sum_{uv\in E(G^{+k})} ts_{G^{+k}}(u) ts_{G^{+k}}(v) \\
&= \sum_{uv\in E_1} ts_{G^{+k}}(u) ts_{G^{+k}}(v) + \sum_{uv\in E_2} ts_{G^{+k}}(u) ts_{G^{+k}}(v) \\
&= \sum_{uv\in E_1} (2nk - 2 + k\sigma_G(v))(nk + k\sigma_G(v)) \\
&\quad + \sum_{uv\in E_2} (nk + k\sigma_G(u))(nk + k\sigma_G(v)) \\
&= \sum_{uv\in E_1} \left(2n^2k^2 - 2nk + (3nk^2 - 2k)\sigma_G(v) + k^2(\sigma_G(v))^2\right) \\
&\quad + \sum_{uv\in E_2} \left(n^2k^2 + nk^2(\sigma_G(u) + \sigma_G(v)) + k^2(\sigma_G(u)\sigma_G(v))\right) \\
&= nk(2n^2k^2 - 2nk) + k(3nk^2 - 2k) \sum_{v\in V(G)} \sigma_G(v) + k^3 \sum_{v\in V(G)} (\sigma_G(v))^2 \\
&\quad + mn^2k^2 + nk^2 \sum_{uv\in E(G)} (\sigma_G(u) + \sigma_G(v)) + k^2 \sum_{uv\in E(G)} \sigma_G(u)\sigma_G(v) \\
&= 2n^2k^2(nk-1) + 2k^2(3nk-2)W(G) + k^3 \sum_{v\in V(G)} (\sigma_G(v))^2 \\
&\quad + mn^2k^2 + nk^2 S_1(G) + k^2 S_2(G).
\end{aligned}$$

$\square$

For a graph G with $diam(G) \leq 2$ [24],

$$\begin{aligned} \sigma_G(v) &= 2n - 2 - d_G(u), \\ S_1(G) &= 4m(n-1) - M_1(G), \\ S_2(G) &= 4m(n-1)^2 - 2(n-1)M_1(G) + M_2(G). \end{aligned}$$

Substituting these in Theorem 9 we get the next corollary.

Corollary 3. *Let G be a graph on n vertices and m edges and let $diam(G) \leq 2$. Then for $k \geq 1$*

$$TS_1(G^{+k}) = nk(3nk-2) + 2mnk + 4mk(n-1) - M_1(G) + 4nk^2(n-1) - 2m$$

and

$$\begin{aligned} TS_2(G^{+k}) &= 2n^2k^2(nk-1) + k(3nk^2 - 2k)\left(2n(n-1) - 2m\right) \\ &+k^3\left(4n(n^2-2n+1) - 8m(n-1) + M_1(G)\right) + mn^2k^2 \\ &+4mnk^2(n-1) - M_1(G) + k^2\left(4m(n-1)^2 - 2(n-1)M_1(G) + M_2(G)\right). \end{aligned}$$

Corollaries 4 to 7 are straightforward from the Corollary 3.

Corollary 4. *Let K_n be a complete graph on n vertices and m edges. Then*

$$TS_1(K_n^{+k}) = nk(3nk-2) + 2mnk + kn(n-1)^2 + 2k^2n(n-1)$$

and

$$\begin{aligned} TS_2(K_n^{+k}) &= 2n^2k^2(nk-1) + k^2n(n-1)(3nk-2) + k^3n(n-1)^2 + mn^2k^2 \\ &+nk^2(n-1)^2 + \frac{k^2}{2}n(n-1)^3. \end{aligned}$$

Corollary 5. *Let $K_{p,q}$ be the complete bipartite graph on $n = p+q$ vertices and $m = pq$ edges. Then*

$$TS_1(K_{p,q}^{+k}) = nk(3nk-2) + 2mnk + kpq(3p+3q-4) + 4k^2(p^2+q^2+pq-p-q)$$

and

$$\begin{aligned} TS_2(K_{p,q}^{+k}) &= 2n^2k^2(nk-1) + 2k(3nk^2-2k)(p^2+q^2+pq-p-q) \\ &+k^3[p(q+2p-2)^2 + q(p+2q-2)^2] + mn^2k^2 \\ &+nk^2pq(3p+3q-4) + k^2pq(2(p+q-1)(p+q-2)+pq). \end{aligned}$$

A *wheel* W_{n+1} is a graph obtained from the cycle C_n, $n \geq 3$, by adding a new vertex and making it adjacent to all the vertices of C_n.

Corollary 6. *Let W_{n+1} be the wheel on $n+1$ vertices and m edges. Then*

$$TS_1(W_{n+1}^{+k}) = nk(3nk-2) + 2mnk + k(7n^2 - 9n) + 4k^2 n(n-1)$$

and

$$\begin{aligned} TS_2(W_{n+1}^{+k}) \;=\; & 2n^2k^2(nk-1) + 2kn(3nk^2 - 2k)(n-1) + nk^3(4n^2 - 11n + 9). \\ & + mn^2k^2 + nk^2(7n^2 - 9n) + k^2(6n^3 - 15n^2 + 9n). \end{aligned}$$

A *windmill graph* F_n, $n \geq 2$, is a graph that can be constructed by coalescence n copies of the cycle C_3 of length 3 with a common vertex. It has $2n+1$ vertices and $3n$ edges.

Corollary 7. *Let F_n be the windmill graph on $2n+1$ vertices and m edges. Then*

$$TS_1(F_n^{+k}) = nk(3nk-2) + 2mnk + k(20n^2 - 8n) + 4nk^2(4n-1)$$

and

$$\begin{aligned} TS_2(F_n^{+k}) \;=\; & 2n^2k^2(nk-1) + 2nk(3nk^2 - 2k)(4n-1) + 4nk^3(8n^2 - 7n + 2) \\ & + mn^2k^2 + nk^2(20n^2 - 8n) + k^2(32n^3 - 24n^2 + 4n). \end{aligned}$$

Corollaries 8 and 9 follows from the Theorem 9.

Corollary 8. *Let P_n be a path on n vertices. Then*

$$TS_1(P_n^{+k}) = nk(3nk-2) + 2mnk + \frac{k}{3}n(n-1)(2n-1) + 4k^2 W(P_n)$$

and

$$\begin{aligned} TS_2(P_n^{+k}) \;=\; & 2n^2k^2(nk-1) + 2k(3nk^2 - 2k)W(P_n) + k^3 \sum_{v \in V(P_n)} (\sigma_{P_n}(v))^2 + mn^2k^2 \\ & + \frac{n^2k^2}{3}(n-1)(2n-1) \\ & + k^2 \left[\frac{(n-1)(n^4 - n^2)}{4} - \frac{n(n-1)(n^3 - n)}{2} + \frac{n(n-1)(2n-1)(2n^2-1)}{6} \right] \\ & - k^2 \left[\frac{n^3(n-1)^2}{2} - \frac{1}{30}(6(n-1)^5 + 15(n-1)^4 - 10(n-1)^3 + (n-1)) \right]. \end{aligned}$$

Corollary 9. *Let C_n be a cycle on $n \geq 3$ vertices.*
(i) *If n is even, then*

$$TS_1(C_n^{+k}) = nk(3nk-2) + 2mnk + \frac{kn^3}{2} + \frac{k^2n^3}{2}$$

and

$$TS_2(C_n^{+k}) = 2n^2k^2(nk-1) + (3nk^2-2k)\frac{k^3n^3}{2} + \frac{k^3n^5}{16} + mn^2k^2 + \frac{n^4k^2}{2} + \frac{n^5k^2}{16}.$$

(ii) *If n is odd, then*

$$TS_1(C_n^{+k}) = nk(3nk-2) + 2mnk + \frac{kn(n^2-1)}{2} + \frac{k^2n(n^2-1)}{2}$$

and

$$\begin{aligned} TS_2(C_n^{+k}) &= 2n^2k^2(nk-1) + (3nk^2-2k)\frac{nk(n^2-1)}{4} + \frac{k^3n(n^2-1)^2}{16} \\ &\quad + mn^2k^2 + \frac{n^2k^2(n^2-1)}{2} + \frac{nk^2(n^2-1)^2}{16}. \end{aligned}$$

Theorem 10. *Let G be a connected graph with $n \geq 3$ vertices, m edges and n_t pendent vertices. Let $diam(G) = D$. Then*

$$n_t(2m + n_t - 2) \leq TS_1(G) \leq n_t(2Dm - D - n_t)$$

and

$$n_t^2(m + n_t - 2) \leq TS_2(G) \leq Dn_t^2(Dm - D - n_t + 1).$$

Proof. The edge set $E(G)$ of a graph G can be partitioned into two sets E_1 and E_2, where $E_1 = \{uv \mid d_G(u) = 1 \text{ and } d_G(v) > 1\}$ and $E_2 = \{uv \mid d_G(u) > 1 \text{ and } d_G(v) > 1\}$. It is easy to check that $|E_1| = n_t$ and $|E_2| = m - n_t$.

We first prove the lower bound. If $uv \in E_1$, then $ts_G(u) \geq 2(n_t - 1)$ and $ts_G(v) \geq n_t$. If $uv \in E_2$, then $ts_G(u) \geq n_t$ and $ts_G(v) \geq n_t$. Therefore

$$\begin{aligned} TS_1(G) &= \sum_{uv \in E(G)} [ts_G(u) + ts_G(v)] \\ &= \sum_{uv \in E_1} [ts_G(u) + ts_G(v)] + \sum_{uv \in E_2} [ts_G(u) + ts_G(v)] \\ &\geq \sum_{uv \in E_1} [2(n_t - 1) + n_t] + \sum_{uv \in E_2} [n_t + n_t] \\ &= n_t(3n_t - 2) + (m - n_t)(2n_t) \\ &= n_t(2m + n_t - 2) \end{aligned}$$

and

$$\begin{aligned}
TS_2(G) &= \sum_{uv\in E(G)} ts_G(u)ts_G(v)] \\
&= \sum_{uv\in E_1} ts_G(u)ts_G(v) + \sum_{uv\in E_2} ts_G(u)ts_G(v) \\
&\geq \sum_{uv\in E_1} 2(n_t-1)n_t + \sum_{uv\in E_2} (n_t)(n_t) \\
&= 2n_t^2(n_t-1)+(m-n_t)(n_t^2) \\
&= n_t^2(m+n_t-2).
\end{aligned}$$

Next we prove the upper bound. If $uv \in E_1$, then $ts_G(u) \leq D(n_t-1)$ and $ts_G(v) \leq (D-1)n_t$. If $uv \in E_2$, then $ts_G(u) \leq Dn_t$ and $ts_G(v) \leq Dn_t$. Therefore

$$\begin{aligned}
TS_1(G) &= \sum_{uv\in E(G)} [ts_G(u)+ts_G(v)] \\
&= \sum_{uv\in E_1} [ts_G(u)+ts_G(v)] + \sum_{uv\in E_2} [ts_G(u)+ts_G(v)] \\
&\leq \sum_{uv\in E_1} [D(n_t-1)+(D-1)n_t] + \sum_{uv\in E_2} [Dn_t+Dn_t] \\
&= n_t(2Dn_t-D-n_t)+(m-n_t)(2Dn_t) \\
&= n_t(2Dm-D-n_t)
\end{aligned}$$

and

$$\begin{aligned}
TS_2(G) &= \sum_{uv\in E(G)} ts_G(u)ts_G(v) \\
&= \sum_{uv\in E_1} ts_G(u)ts_G(v) + \sum_{uv\in E_2} ts_G(u)ts_G(v) \\
&\leq \sum_{uv\in E_1} D(n_t-1)(D-1)n_t + \sum_{uv\in E_2} (Dn_t)(Dn_t) \\
&= Dn_t^2(n_t-1)(D-1)+(m-n_t)D^2n_t^2 \\
&= Dn_t^2(Dm-D-n_t+1).
\end{aligned}$$

□

4. Regression analysis

In this section we investigate and discuss the correlation of boiling point (BP) and critical temperature (CT) of the cycloalkanes with the topological indices based on the degrees and distances.

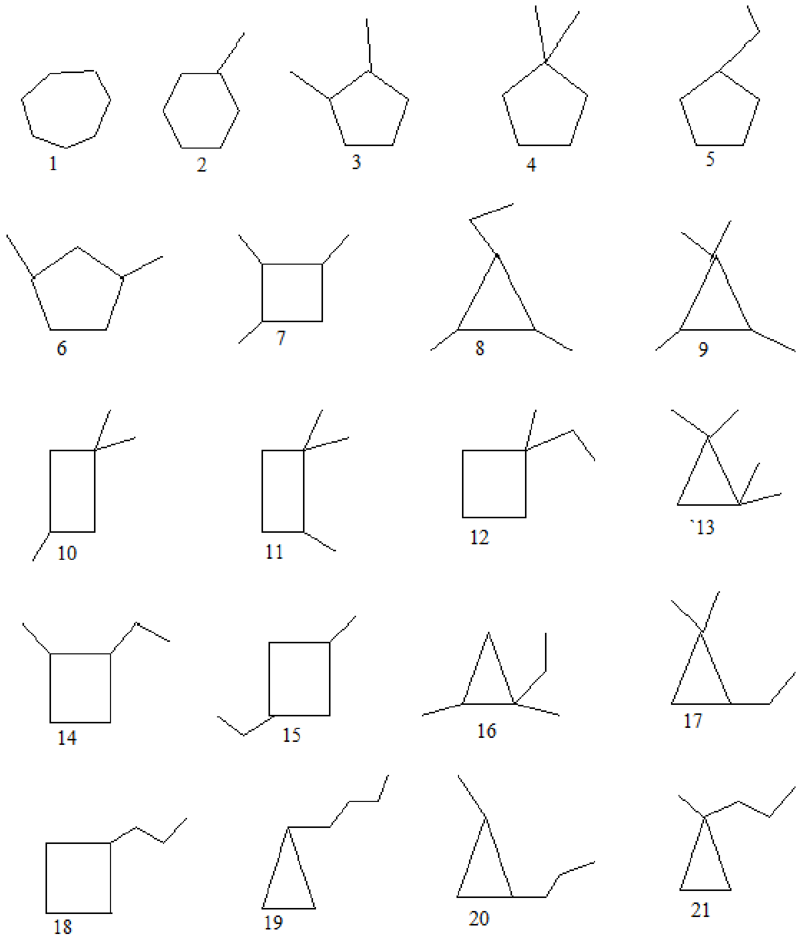

Figure 3. Molecular structure of Cycloalkanes

Experimental values of the boiling point and critical temperature of the cycloalkanes are given in Table 1.

The scatter plots of BP and CT with the indices M_1, M_2, S_1, S_2, W, TW, TS_1 and TS_2 are shown in Figs. 4 to 19.

The linear regression models for the boiling point (BP) using the data of Table 1 are obtained using the least square fitting procedure as implimented in Eqs. (4) to (11).

Table 1. **Physical properties and indices of Cycloalkanes**

Sl. No.	Cycloalkanes	BP in [K]	CT in [K]	M_1	M_2	S_1	S_2	W	TW	TS_1	TS_2
1	cyclo heptane	388.25	601.57	28	28	168	1008	42	0	0	0
2	3-methyl cyclohexane	379.31	583	30	31	163	946	42	0	31	40
3	1,2-dimethyl cyclopentane	370.37	564.59	32	35	150	705	40	3	56	117
4	1,1-dimethyl cyclopentane	375.28	562.9	34	36	146	752	39	2	52	108
5	ethyl cyclopentane	375.04	573.36	30	32	164	965	43	0	36	54
6	1,3-dimethyl cyclopentane	370.37	564.59	32	34	154	841	41	4	60	129
7	1,2,3-trimethyl cyclobutane	361.43	546.33	32	39	153	826	42	10	85	258
8	1-ethyl-2,3-dimethyl cyclopropane	357.16	537.31	34	41	158	892	44	11	90	290
9	1,1,2,3-tetramethyl cyclopropane	366.34	544.19	38	48	140	688	40	16	100	355
10	1,1,3-trimethyl cyclobutane	366.34	544.19	36	39	153	828	42	10	85	260
11	1,1,2-trimethyl cyclobutane	366.34	544.19	36	41	145	734	40	8	81	214
12	1-ethyl-1-methyl cyclobutane	371.01	553.3	34	38	155	852	42	3	58	127
13	1,1,2,2-tetramethyl cyclopropane	362.31	523.08	40	48	136	640	39	16	96	324
14	1-ethyl-2-methyl cyclobutane	366.1	555.27	32	36	163	946	44	4	64	148
15	1-ethyl-3-methyl cyclobutane	366.1	555.27	32	35	171	1052	46	5	70	175
16	1-ethyl-1,2-dimethyl cyclopropane	362.07	534.91	36	39	150	796	42	10	84	251
17	2-ethyl-1,1-dimethyl cyclopropane	362.07	534.91	36	42	154	843	43	10	86	265
18	propyl cyclobutane	370.77	564.05	30	32	183	1208	48	0	41	72
19	butyl cyclopropane	366.5	555.06	30	32	186	1384	51	0	44	85
20	1-methyl-2-propyl cyclopropane	361.83	546.26	32	36	178	1140	48	5	72	185
21	1-methyl-1-propyl cyclopropane	366.74	544.02	34	38	166	983	45	4	64	148

Table 2. **Correlation coefficient (R) between indices and properties of cycloalkanes.**

Index	Boiling point (BP)	Critical temparature (CT)
M_1	0.647	0.862
M_2	0.769	0.909
S_1	0.248	0.445
S_2	0.193	0.369
W	0.111	0.084
TW	0.764	0.851
TS_1	0.922	0.950
TS_2	0.871	0.920

$$BP = 420.850(\pm 14.427) - 1.598(\pm 0.432)M_1 \tag{4}$$
$$BP = 409.073(\pm 7.949) - 1.113(\pm 0.212)M_2 \tag{5}$$
$$BP = 345.825(\pm 19.688) + 0.138(\pm 0.124)S_1 \tag{6}$$
$$BP = 345.825(\pm 19.688) + 0.138(\pm 0.124)S_2 \tag{7}$$
$$BP = 379.001(\pm 23.141) - 0.262(\pm 0.537)W \tag{8}$$
$$BP = 374.146(\pm 1.638) - 1.110(\pm 0.215)TW \tag{9}$$
$$BP = 385.518(\pm 1.830) - 0.275(\pm 0.027)TS_1 \tag{10}$$
$$BP = 379.025(\pm 1.670) - 0.066(\pm 0.008)TS_2 \tag{11}$$

From Table 2, the model (10) shows that the correlation of the boiling point of the cycloalkanes with first terminal status connectivity index is better ($R = 0.950$) than the correlation with other degree and distance based topological indices considered in this paper.
The linear regression models for the critical temperature (CT) using the data of Table 1 are given in Eqs. (12) to (19).

$$CT = 732.329(\pm 24.326) - 5.394(\pm 0.729)M_1 \tag{12}$$
$$CT = 676.734(\pm 13.165) - 3.330(\pm 0.351)M_2 \tag{13}$$
$$CT = 453.479(\pm 46.124) + 0.0.627(\pm 0.289)S_1 \tag{14}$$
$$CT = 518.722(\pm 20.227) + 0.038(\pm 0.022)S_2 \tag{15}$$
$$CT = 531.575(\pm 58.798) + 0.499(\pm 1.364)W \tag{16}$$
$$CT = 571.086(\pm 3.381) - 3.132(\pm 0.444)TW \tag{17}$$
$$CT = 599.449(\pm 3.723) - 0.719(\pm 0.054)TS_1 \tag{18}$$
$$CT = 583.206(\pm 3.378) - 0.176(\pm 0.017)TS_2 \tag{19}$$

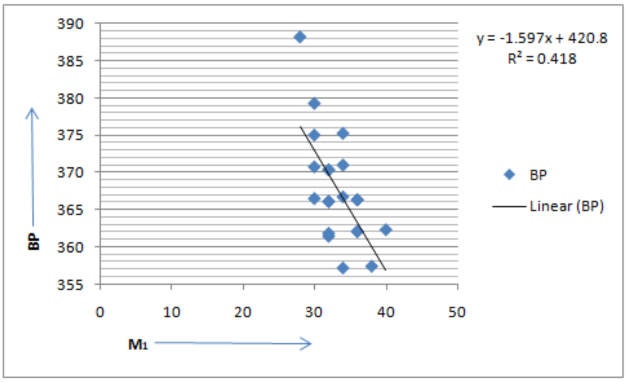

Figure 4. **Scatter plot between BP and M_1.**

From Table 2, the model (18) shows that the correlation of the critical temperature of the cycloalkanes with first terminal status connectivity index is better ($R = 0.922$) than the correlation with other topological indices.

5. Conclusion

The terminal status of a vertex and terminal status connectivity indices are introduced and obtained these for some graphs. Also obtained the bounds for these parameters. Further a regression analysis of the boiling point and critical temperature of the cycloalkanes with the distance based indices has been carried out and compared the linear models. The linear model obtained, based on the first terminal status connectivity index, is better than the models based on the other indices.

Acknowledgements

The author K. Bhajantri is thankful to Karnataka Science and Technology Promotion Society, Bengaluru for fellowship No. DST/KSTePS/Ph.D. Fellowship/OTH-02: 2019-20.

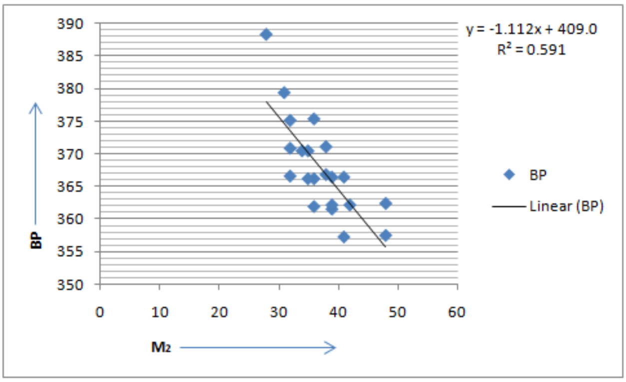

Figure 5. **Scatter plot between BP and M_2.**

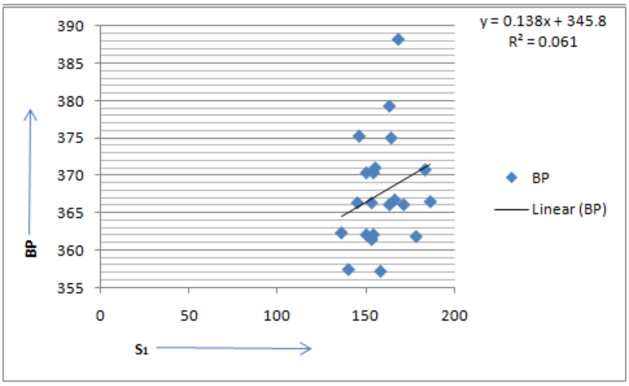

Figure 6. **Scatter plot between BP and S_1.**

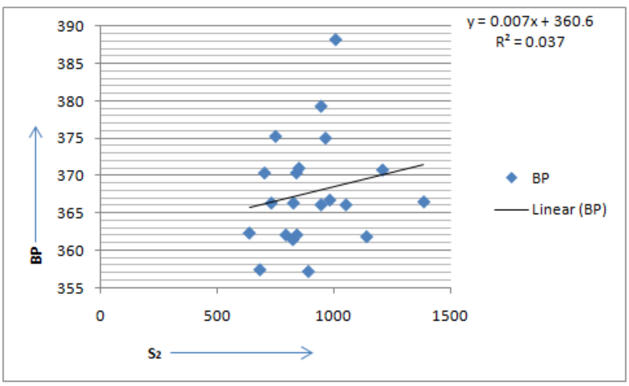

Figure 7. **Scatter plot between BP and S_2.**

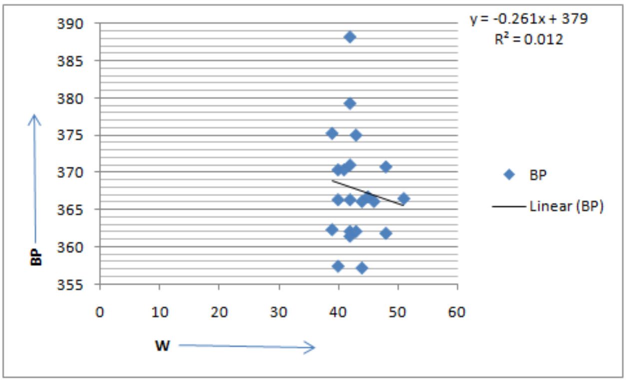

Figure 8. **Scatter plot between** BP **and** W,

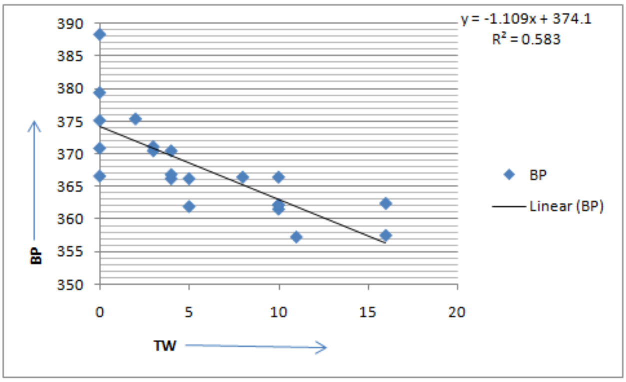

Figure 9. **Scatter plot between** BP **and** TW.

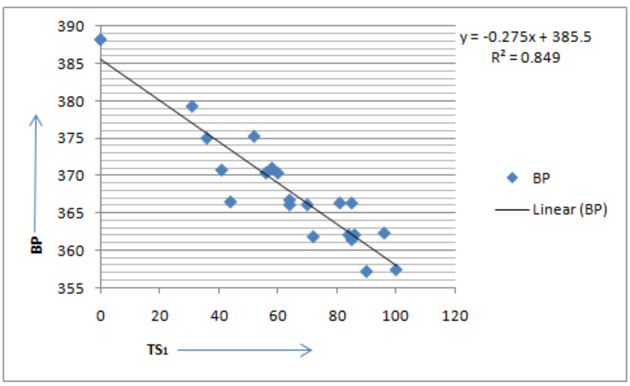

Figure 10. **Scatter plot between** BP **and** TS_1.

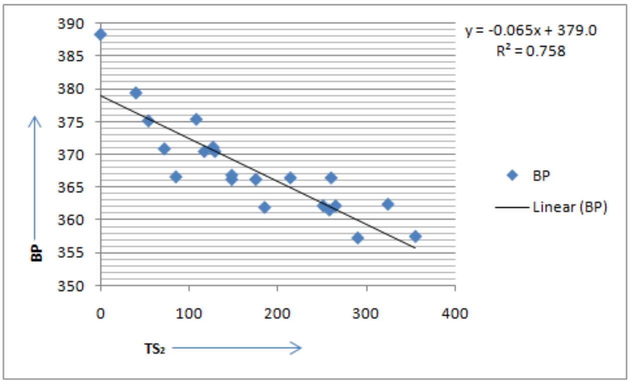

Figure 11. **Scatter plot between BP and TS_2.**

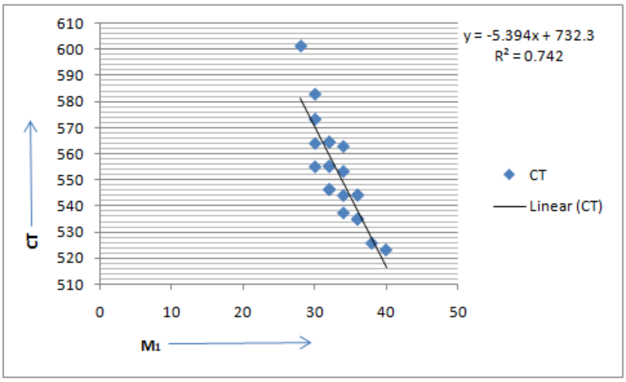

Figure 12. **Scatter plot between CT and M_1.**

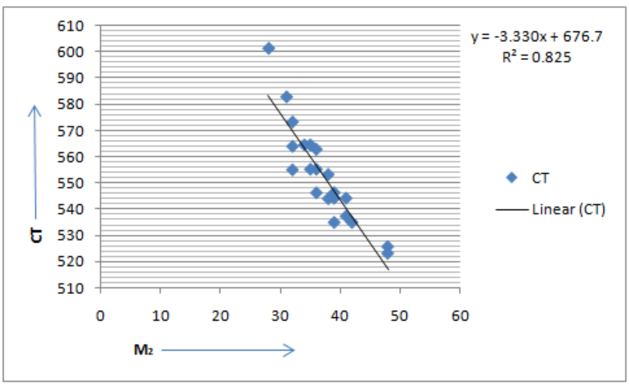

Figure 13. **Scatter plot between CT and M_2.**

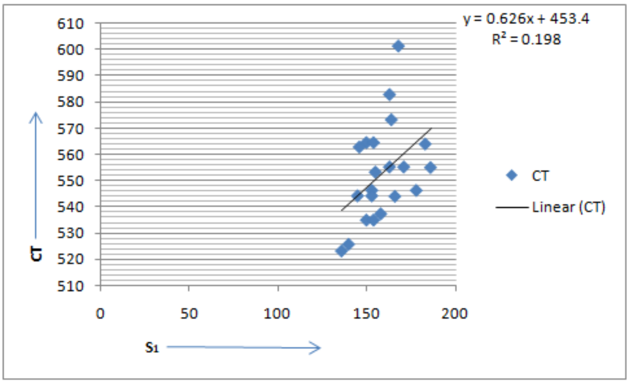

Figure 14. **Scatter plot between** CT **and** S_1.

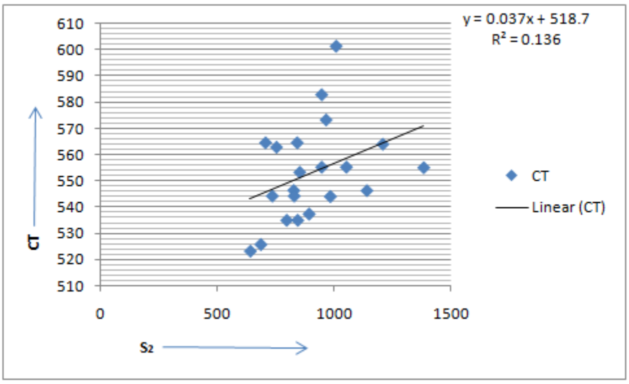

Figure 15. **Scatter plot between** CT **and** S_2.

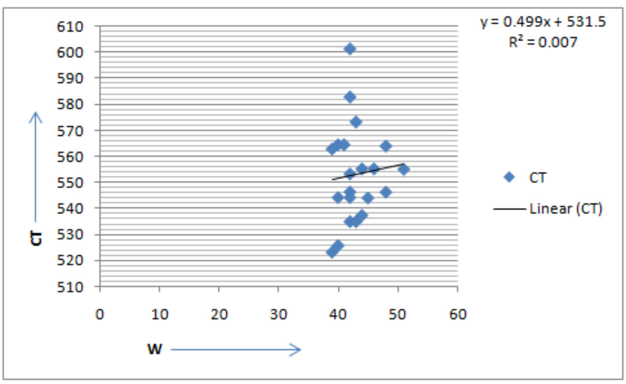

Figure 16. **Scatter plot between** CT **and** W.

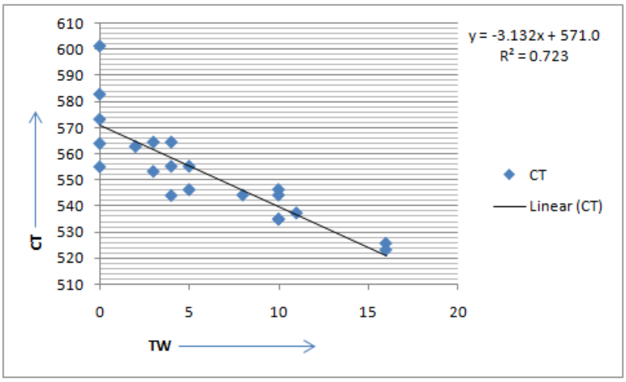

Figure 17. **Scatter plot between CT and TW.**

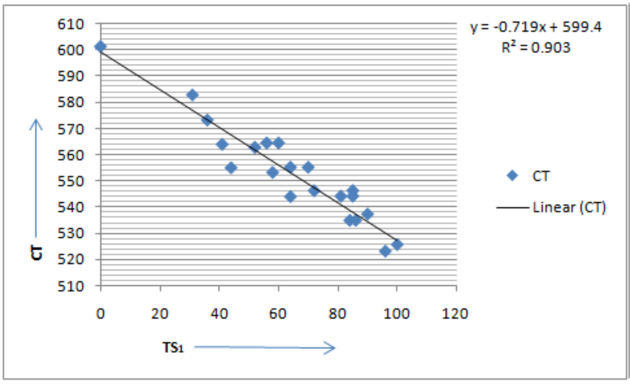

Figure 18. **Scatter plot between CT and TS_1.**

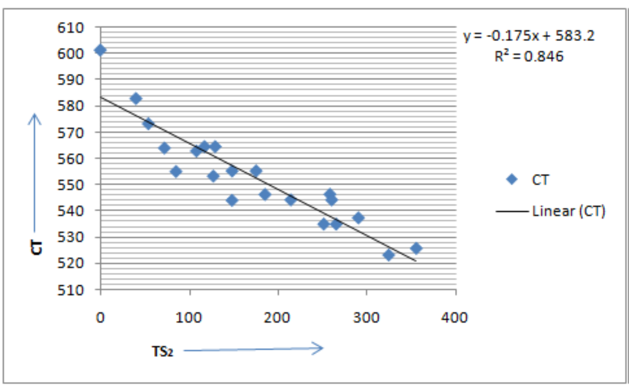

Figure 19. **Scatter plot between CT and TS_2.**

References

[1] A.R. Ashrafi and M. Ghorbani, *Eccentric connectivity index of fullerenes*, Novel Molecular Structure Descriptors-Theory and Applications II (I. Gutman and B. Furtula, eds.), Uni. Kragujevac, Kragujevac, 2010, pp. 183–192.

[2] X. Deng and J. Zhang, *Equiseparability on terminal Wiener index*, Algorithmic Aspects in Information and Management (A.V. Goldberg and Y. Zhou, eds.), Springer, Berlin, 2009, pp. 166–174.

[3] A.A. Dobrynin, R. Entringer, and I. Gutman, *Wiener index of trees: theory and applications*, Acta Appl. Math. **66** (2001), no. 3, 211–249.

[4] A.A. Dobrynin, I. Gutman, S. Klavžar, and P. Žigert, *Wiener index of hexagonal systems*, Acta Appl. Math. **72** (2002), no. 3, 247–294.

[5] A.A. Dobrynin and A.A. Kochetova, *Degree distance of a graph: A degree analog of the Wiener index*, J. Chem. Inf. Comput. Sci. **34** (1994), no. 5, 1082–1086.

[6] Z. Du, A. Jahanbai, and S.M. Sheikholeslami, *Relationships between Randić index and other topological indices*, Commun. Comb. Optim. **6** (2021), no. 1, 137–154.

[7] I. Gutman, *Selected properties of the Schultz molecular topological index*, J. Chem. Inf. Comput. Sci. **34** (1994), no. 5, 1087–1089.

[8] I. Gutman and B. Furtula, *A survey on terminal Wiener index*, Novel Molecular Structure Descriptors-Theory and Applications I (I. Gutman and B. Furtula, eds.), Uni. Kragujevac, Kragujevac, 2010, pp. 173–190.

[9] ———, *Distance in Molecular Graphs Theory*, Univ. Kragujevac, Kragujevac, 2012.

[10] ———, *Novel Molecular Structure Descriptors-Theory and Application I*, Univ. Kragujevac, Kragujevac, 2012.

[11] I. Gutman, B. Furtula, K.C. Das, E. Milovanović, and I. Milovanović, *Bounds in chemical graph theory-basics*, Univ. Kragujevac, Kragujevac, 2017.

[12] I. Gutman, B. Furtula, and M. Petrović, *Terminal Wiener index*, J. Math. Chem. **46** (2009), no. 2, 522–531.

[13] I. Gutman, B. Ruščić, N. Trinajstić, and C.F. Wilcox Jr, *Graph theory and molecular orbitals. XII. Acyclic polyenes*, J. Chem. Phys. **62** (1975), no. 9, 3399–3405.

[14] I. Gutman, Y.-N. Yeh, S.-L. Lee, and Y.-L. Luo, *Some recent results in the theory of the Wiener number*, Indian J. Chem. **32A** (1993), 651–661.

[15] Ivan Gutman and Nenad Trinajstić, *Graph theory and molecular orbitals. Total φ-electron energy of alternant hydrocarbons*, Chem. Phys. Lett. **17** (1972), no. 4, 535–538.

[16] A. Heydari and I. Gutman, *On the terminal Wiener index of thorn graphs*, Kragujevac J. Sci. **32** (2010), 57–64.

[17] B. Horvat, T. Pisanski, and M. Randic, *Terminal polynomials and star-like graphs*, MATCH Commun. Math. Comput. Chem. **60** (2008), no. 2, 493–512.

[18] I.r Milovanović, M. Matejić, E. Milovanović, and R. Khoeilar, *A note on the first*

Zagreb index and coindex of graphs, Commun. Comb. Optim. **6** (2021), no. 1, 41–51.

[19] T.A. Naikoo, B.A. Rather, U. Samee, and S. Pirzada, *On Zagreb index of tournaments*, Kragujevac J. Math. **48** (2024), no. 2, 241–253.

[20] S. Nikolić and N. Trinajstić, *The Wiener index: Development and applications*, Croat. Chem. Acta **68** (1995), no. 1, 105–129.

[21] M. Pal, S. Samanta, and A. Pal, *Handbook of Research on Advanced Applications of Graph Theory in Modern Society*, IGI Global, Hershey PA, USA, 2020.

[22] S. Pirzada, B.A. Rather, T.A. Naikoo, and T.A. Chishti, *On first general Zagreb index of tournaments*, Creative Math. Inf. (to appear).

[23] H.S. Ramane, K.P. Narayankar, S.S. Shirkol, and A.B. Ganagi, *Terminal Wiener index of line graphs*, MATCH Commun. Math. Comput. Chem. **69** (2013), no. 3, 775–782.

[24] H.S. Ramane and A.S. Yalnaik, *Status connectivity indices of graphs and its applications to the boiling point of benzenoid hydrocarbons*, J. Appl. Math. Comput. **55** (2017), no. 1, 609–627.

[25] H.S. Ramane, A.S. Yalnaik, and R. Sharafdini, *Status connectivity indices and co-indices of graphs and its computation to some distance-balanced graphs*, AKCE Int. J. Graphs Combin. **17** (2020), no. 1, 98–108.

[26] M. Randic, *Characterization of molecular branching*, J. Am. Chem. Soc. **97** (1975), no. 23, 6609–6615.

[27] M. Randić and J. Zupan, *Highly compact 2D graphical representation of DNA sequences*, SAR and QSAR in Environ. Res. **15** (2004), no. 3, 191–205.

[28] M. Randić, J. Zupan, and D. Vikić-Topić, *On representation of proteins by star-like graphs*, J. Mol. Graph. Modell. **26** (2007), no. 1, 290–305.

[29] N.S. Schmuck, S.G. Wagner, and H. Wang, *Greedy trees, caterpillars, and Wiener-type graph invariants*, MATCH Commun. Math. Comput. Chem. **68** (2012), no. 1, 273–292.

[30] L.A. Székely, H. Wang, and T. Wu, *The sum of the distances between the leaves of a tree and the 'semi-regular' property*, Discrete Math. **311** (2011), no. 13, 1197–1203.

[31] R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim, 2000.

[32] D. Vukičević and A. Graovac, *Note on the comparison of the first and second normalized Zagreb eccentricity indices.*, Acta Chim. Slov. **57** (2010), no. 3, 524–528.

[33] H.B. Walikar, H.S. Ramane, and V.S. Shigehalli, *Wiener number of dendrimers*, Proc. Nat. Conf. Math. Comput. Mod. (R. Nadarajan and G. Arulmozhi, eds.), Allied Publishers, New Delhi, 2003, pp. 361–368.

[34] H.B. Walikar, V.S. Shigehalli, and H.S. Ramane, *Bounds on the Wiener number of a graph*, MATCH Commun. Math. Comput. Chem. **50** (2004), no. 1, 117–132.

[35] H. Wiener, *Structural determination of paraffin boiling points*, J. Am. Chem. Soc. **69** (1947), no. 1, 17–20.