



Original article

The Eccentricity Temperature Based Indices of a Graph

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Abstract:

Topological indices in graph theory are numerical parameters associated with a graph that capture structural information about it. These indices play an important role in chemical graph theory, network analysis, and mathematics for comparing graphs and predicting their properties. In this paper, we introduce the eccentricity temperature-based indices of a graph G , namely the sum eccentricity-temperature index $SET(G)$, product eccentricity-temperature index $PET(G)$, and difference eccentricity-temperature index $DET(G)$. We determine the exact values of these indices for certain classes of graphs and establish several bounds and characterizations by applying classical inequalities. Also, we obtain the comparative analysis among the eccentricity temperature based graphical indices of molecular graphs of octane isomers.

Keywords: generalised sum, product and difference based Eccentricity Harary indices,

Introduction:

Throughout this paper, we considered simple, finite, connected, undirected, without loops or multiple edge graphs. Assume that G is a connected graph with $|V(G)| = p$ vertices and $|E(G)| = q$ edges. The maximum and minimum degree of the graphs represented by $\Delta(G)$ and $\delta(G)$ respectively. For a vertex $v \in V(G)$ and $d(v)$ denotes the degree of v . For any $u, v \in V(G)$, the distance $d(u, v)$ is defined as the length of shortest path between u and v . Eccentricity is the vertex u from the farthest vertex in G . that is

$$e(u) = \max\{d(u, v) / \forall u \in V(G)\}$$



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The minimum eccentricity is called radius, $r(G)$ and maximum eccentricity is called diameter, $diam(G)$. For basic graph-theoretical terminology and notation we follow [4].

Fajtlowicz [3] defined the temperature of any vertex $v \in V(G)$, where $V(G)$ is vertex set and $|V(G)| = n$ is the total number of vertices of G , then

$$T(u) = \frac{d_G(u)}{n - d_G(u)}$$

For more information to temperature based indices and its applications, we refer to [5, 8, 9, 10]

We initiate the novel distance and temperature based topological indices of a connected graph are defined as follows

The sum eccentricity temperature index of a graph G is defined as

$$SET(G) = \sum_{\{u,v\} \subseteq V(G)} T_e(u) + T_e(v)$$

The product eccentricity temperature index of a graph G is defined as

$$PET(G) = \sum_{\{u,v\} \subseteq V(G)} T_e(u) \cdot T_e(v)$$

The difference eccentricity temperature index of a graph G is defined as

$$DET(G) = \sum_{\{u,v\} \subseteq V(G)} |T_e(u) - T_e(v)|$$

where $T_e(u)$ is the eccentricity temperature of a vertex u and is defined as follows

$$T_e(u) = \frac{e(u)}{p - e(u)}$$

where $e(u)$ is eccentricity of a vertices and p is the number vertices of a graph.

Eccentricity temperature based indices of some classical graphs

Theorem 1.1. Let G be a cycle with vertices $p \geq 3$, then

$$\begin{aligned} SET(C_p) &= p(p-1) \left\{ \frac{\lfloor p/2 \rfloor}{p - \lfloor p/2 \rfloor} \right\} \\ PET(C_p) &= \frac{p(p-1)}{2} \left\{ \frac{\lfloor p/2 \rfloor}{p - \lfloor p/2 \rfloor} \right\}^2 \\ DET(C_p) &= 0 \end{aligned}$$

Proof. Let G be a cycle with $p \geq 3$ vertices. The eccentricity of the every vertex in cycle is $\lfloor p/2 \rfloor$. i.e., $e(u) = \lfloor p/2 \rfloor$.

We know that

$$\begin{aligned} T_e(u) &= \frac{e(u)}{p - e(u)} \\ T_e(u) &= \frac{\lfloor p/2 \rfloor}{p - \lfloor p/2 \rfloor} \end{aligned}$$

where $e(u) = \lfloor p/2 \rfloor$, and p represents the number of vertices

The sum of eccentricity temperature is given by

$$\begin{aligned}
 SET(C_p) &= \sum_{\{u,v\} \subseteq V(G)} (T_e(u) + T_e(v)) \\
 &= \sum_{\{u,v\} \subseteq V(G)} \left(\frac{e(u)}{p - e(u)} + \frac{e(v)}{p - e(v)} \right) \\
 &= \sum_{\{u,v\} \subseteq V(G)} \left(\frac{\lfloor p/2 \rfloor}{p - \lfloor p/2 \rfloor} + \frac{\lfloor p/2 \rfloor}{p - \lfloor p/2 \rfloor} \right) \\
 SET(C_p) &= p(p - 1) \left\{ \frac{\lfloor p/2 \rfloor}{p - \lfloor p/2 \rfloor} \right\}
 \end{aligned}$$

The product of eccentricity temperature is given by

$$\begin{aligned}
 PET(C_p) &= \sum_{\{u,v\} \subseteq V(G)} T_e(u) \cdot T_e(v) \\
 &= \sum_{\{u,v\} \subseteq V(G)} \left(\frac{e(u)}{p - e(u)} \cdot \frac{e(v)}{p - e(v)} \right) \\
 &= \sum_{\{u,v\} \subseteq V(G)} \frac{\lfloor p/2 \rfloor}{p - \lfloor p/2 \rfloor} \cdot \frac{\lfloor p/2 \rfloor}{p - \lfloor p/2 \rfloor} \\
 PET(C_p) &= \frac{p(p - 1)}{2} \left\{ \frac{\lfloor p/2 \rfloor}{p - \lfloor p/2 \rfloor} \right\}^2
 \end{aligned}$$

The difference of eccentricity temperature is given by

$$\begin{aligned}
 DET(C_p) &= \sum_{\{u,v\} \subseteq V(G)} |(T_e(u) - T_e(v))| \\
 &= \sum_{\{u,v\} \subseteq V(G)} \left| \left(\frac{e(u)}{p - e(u)} - \frac{e(v)}{p - e(v)} \right) \right| \\
 &= \sum_{\{u,v\} \subseteq V(G)} \frac{\lfloor p/2 \rfloor}{p - \lfloor p/2 \rfloor} - \frac{\lfloor p/2 \rfloor}{p - \lfloor p/2 \rfloor} \\
 DET(C_p) &= 0
 \end{aligned}$$

Theorem 1.2. Let G be a complete graph with vertices $p \geq 3$, then

$$\begin{aligned}
 SET(K_p) &= p \\
 PET(K_p) &= \frac{p}{2(p - 1)} \\
 DET(K_p) &= 0
 \end{aligned}$$

Proof. Let G be a complete graph with $p \geq 3$ vertices. The eccentricity of the complete graph is 1. i.e., $e(u) = 1$.

We know that

$$\begin{aligned}
 T_e(u) &= \frac{e(u)}{p - e(u)} \\
 T_e(u) &= \frac{1}{p - 1}
 \end{aligned}$$

where $e(u) = 1$, and p represents the number of vertices. The sum of eccentricity temperature is given by:

$$\begin{aligned}
 SET(K_p) &= \sum_{\{u,v\} \subseteq V(G)} (T_e(u) + T_e(v)) \\
 &= \sum_{\{u,v\} \subseteq V(G)} \left(\frac{e(u)}{p - e(u)} + \frac{e(v)}{p - e(v)} \right) \\
 &= \sum_{\{u,v\} \subseteq V(G)} \left(\frac{1}{p - 1} + \frac{1}{p - 1} \right) \\
 SET(K_p) &= p
 \end{aligned}$$

The product of eccentricity temperature is given by

$$\begin{aligned}
 PET(K_p) &= \sum_{\{u,v\} \subseteq V(G)} (T_e(u) \cdot T_e(v)) \\
 &= \sum_{\{u,v\} \subseteq V(G)} \left(\frac{e(u)}{p - e(u)} \cdot \frac{e(v)}{p - e(v)} \right) \\
 &= \sum_{\{u,v\} \subseteq V(G)} \left(\frac{1}{p - 1} \cdot \frac{1}{p - 1} \right) \\
 &= \frac{p(p - 1)}{2} \left(\frac{1}{p - 1} \right)^2 \\
 PET(K_p) &= \frac{p}{2(p - 1)}
 \end{aligned}$$

The difference of eccentricity temperature is given by

$$\begin{aligned}
 DET(K_p) &= \sum_{\{u,v\} \subseteq V(G)} |(T_e(u) - T_e(v))| \\
 &= \sum_{\{u,v\} \subseteq V(G)} \left| \left(\frac{e(u)}{p - e(u)} - \frac{e(v)}{p - e(v)} \right) \right| \\
 &= \sum_{\{u,v\} \subseteq V(G)} \left(\frac{1}{p - 1} - \frac{1}{p - 1} \right) \\
 DET(K_p) &= 0
 \end{aligned}$$

Theorem 1.3. Let G be a wheel with vertices $p \geq 5$, then

$$\begin{aligned}
 SET(W_p) &= \frac{p(2p - 3)}{p - 2} \\
 PET(W_p) &= \frac{2p}{p - 2} \\
 DET(W_p) &= \frac{p}{p - 2}
 \end{aligned}$$

Proof. Let G be a wheel with $p \geq 5$ vertices. The eccentricity of the wheel is 2 & 1. i.e., $e(u) = 2$, & $e(v) = 1$.

We know that

$$\begin{aligned}
 T_e(u) &= \frac{e(u)}{p - e(u)} \\
 T_e(u) &= \frac{2}{p - 2} + \frac{2}{p - 2} \\
 T_e(u) &= \frac{1}{p - 1} + \frac{2}{p - 2}
 \end{aligned}$$

where $e(u) = 2, e(v) = 1$, and p represents the number of vertices.

The sum of eccentricity temperature is given by

$$\begin{aligned}
 SET(W_p) &= \sum_{\{u,v\} \subseteq V(G)} (T_e(u) + T_e(v)) \\
 &= \sum_{\{u,v\} \subseteq V(G)} \left(\frac{e(u)}{p-e(u)} \right) + \sum_{\{u,v\} \subseteq V(G)} \left(\frac{e(v)}{p-e(v)} \right) \\
 &= \sum_{\{u,v\} \subseteq V(G)} \left(\frac{2}{p-2} + \frac{2}{p-2} \right) + \sum_{\{u,v\} \subseteq V(G)} \left(\frac{1}{p-1} + \frac{2}{p-2} \right) \\
 &= \frac{(p-1)(p-2)}{2} \left(2 \frac{2}{p-2} \right) + (p-1) \left(\frac{p-2+2(p-1)}{(p-2)(p-1)} \right) \\
 &= 2(p-1) + \left(\frac{3p-4}{p-2} \right) \\
 &= \left(\frac{(2p-2)(p-2) + 3p-4}{p-2} \right) \\
 SET(W_p) &= \frac{p(2p-3)}{p-2}
 \end{aligned}$$

The product of eccentricity temperature is given by

$$\begin{aligned}
 PET(W_p) &= \sum_{\{u,v\} \subseteq V(G)} (T_e(u) \cdot T_e(v)) \\
 &= \sum_{\{u,v\} \subseteq V(G)} \left(\frac{e(u)}{p-e(u)} \right) \cdot \left(\frac{e(v)}{p-e(v)} \right) \\
 &= \sum_{\{u,v\} \subseteq V(G)} \left(\frac{2}{p-2} \cdot \frac{2}{p-2} \right) + \sum_{\{u,v\} \subseteq V(G)} \left(\frac{1}{p-1} \cdot \frac{2}{p-2} \right) \\
 PET(W_p) &= \frac{2p}{p-2}
 \end{aligned}$$

The difference of eccentricity temperature is given by

$$\begin{aligned}
 DET(W_p) &= \sum_{\{u,v\} \subseteq V(G)} |(T_e(u) - T_e(v))| \\
 &= \sum_{\{u,v\} \subseteq V(G)} \left| \left(\frac{e(u)}{p-e(u)} \right) - \left(\frac{e(v)}{p-e(v)} \right) \right| \\
 &= \sum_{\{u,v\} \subseteq V(G)} \left| \left(\frac{2}{p-2} - \frac{2}{p-2} \right) \right| + \sum_{\{u,v\} \subseteq V(G)} \left| \left(\frac{1}{p-1} - \frac{2}{p-2} \right) \right| \\
 &= (p-1) \left(\frac{2}{p-2} - \frac{1}{p-1} \right) \\
 DET(W_p) &= \frac{p}{p-2}
 \end{aligned}$$

Theorem 1.4. Let G be a complete bipartite graph $K_{m,n}$, $m, n \geq 2$, then

$$\begin{aligned}
 SET(K_{m,n}) &= mn(mn-1) \left(\frac{2}{m+n-2} \right) \\
 PET(K_{m,n}) &= mn(mn-1) \frac{2}{(m+n-2)^2} \\
 DET(K_{m,n}) &= 0
 \end{aligned}$$

Proof. Let G be a complete bipartite graph with $K_{m,n}$, $m, n \geq 2$, vertices. The eccentricity of each vertex in the complete bipartite graph is 2. i.e., $e(u) = 2$.

We know that

$$T_e(u) = \frac{e(u)}{m+n-e(u)}$$

$$T_e(u) = \frac{2}{m+n-2}$$

where $e(u) = 2$, and p represents the number of vertices.

The sum of eccentricity temperature is given by

$$\begin{aligned} SET(K_{m,n}) &= \sum_{\{u,v\} \subseteq V(G)} T_e(u) + T_e(v) \\ &= \sum_{\{u,v\} \subseteq V(G)} \left(\frac{e(u)}{p-e(u)} + \frac{e(v)}{p-e(v)} \right) \\ &= \sum_{\{u,v\} \subseteq V(G)} \frac{2}{m+n-2} + \frac{2}{m+n-2} \\ SET(K_{m,n}) &= mn(mn-1) \left(\frac{2}{m+n-2} \right) \end{aligned}$$

The product of eccentricity temperature is given by

$$\begin{aligned} PET(K_{m,n}) &= \sum_{\{u,v\} \subseteq V(G)} T_e(u) \cdot T_e(v) \\ &= \sum_{\{u,v\} \subseteq V(G)} \left(\frac{e(u)}{p-e(u)} \cdot \frac{e(v)}{p-e(v)} \right) \\ &= \sum_{\{u,v\} \subseteq V(G)} \left(\frac{2}{m+n-2} \cdot \frac{2}{m+n-2} \right) \\ &= \frac{mn(mn-1)}{2} \left(\frac{2}{m+n-2} \right)^2 \\ PET(K_{m,n}) &= mn(mn-1) \frac{2}{(m+n-2)^2} \end{aligned}$$

By the definition of difference eccentricity temperature index we get

$$\begin{aligned} DET(K_{m,n}) &= \sum_{\{u,v\} \subseteq V(G)} |(T_e(u) - T_e(v))| \\ &= \sum_{\{u,v\} \subseteq V(G)} \left| \left(\frac{e(u)}{p-e(u)} - \frac{e(v)}{p-e(v)} \right) \right| \\ DET(K_{m,n}) &= 0 \end{aligned}$$

Corollary 1.4.1. Let G be a star $S_{1,n}$ with $m = 1$ and $n \geq 3$. Then

$$SET(S_{1,n}) = 2n$$

$$PET(S_{1,n}) = \frac{2n}{n-1}$$

Bounds of the eccentricity temperature of graph indices

Theorem 1.5. Let G be an any graph. Then

$$i) p \leq SET(G) \leq p(p-1)^2$$

$$ii) \frac{p}{2(p-1)} \leq PET(G) \leq \frac{p(p-1)^3}{2}$$

Proof. Let G be any graph. let $e(u)$ be an eccentricity of a graph then the eccentricity is given by

$$\begin{aligned} 1 &\leq e(u) \leq p-1 \\ 1-p &\leq e(u)-p \leq p-1-p \\ 1-p &\leq -(p-e(u)) \leq -1 \\ p-1 &\leq (p-e(u)) \leq 1 \\ \frac{1}{p-1} &\leq \frac{e(u)}{p-e(u)} \leq \frac{p-1}{1} \\ \frac{1}{p-1} &\leq \frac{e(u)}{p-e(u)} \leq (p-1) \\ \frac{2}{p-1} &\leq \frac{e(u)}{p-e(u)} + \frac{e(u)}{p-e(u)} \leq 2p-1 \\ \sum \frac{2}{p-1} &\leq \sum \frac{e(u)}{p-e(u)} + \frac{e(u)}{p-e(u)} \leq \sum 2(p-1) \\ \sum \frac{2}{p-1} &\leq \sum T_e(u) + T_e(u) \leq \sum 2(p-1) \\ \frac{p(p-1)}{2} \cdot \frac{2}{p-1} &\leq SET(G) \leq \frac{p(p-1)}{2} 2(p-1) \\ p &\leq SET(G) \leq p(p-1)^2 \end{aligned}$$

Result (i) follows.

$$\begin{aligned} 1-p &\leq -(p-e(u)) \leq -1 \\ p-1 &\leq (p-e(u)) \leq 1 \\ \frac{1}{p-1} &\leq \frac{e(u)}{p-e(u)} \leq \frac{p-1}{1} \\ \frac{1}{p-1} &\leq \frac{e(u)}{p-e(u)} \leq (p-1) \\ \frac{1}{p-1} \cdot \frac{1}{p-1} &\leq \frac{e(u)}{p-e(u)} \cdot \frac{e(u)}{p-e(u)} \leq (p-1) \cdot (p-1) \\ \left(\frac{1}{p-1}\right)^2 &\leq \frac{e(u)}{p-e(u)} \cdot \frac{e(u)}{p-e(u)} \leq (p-1)^2 \\ \sum \left(\frac{1}{p-1}\right)^2 &\leq \sum \left(\frac{e(u)}{p-e(u)} \cdot \frac{e(u)}{p-e(u)}\right) \leq \sum (p-1)^2 \\ \sum \left(\frac{1}{p-1}\right)^2 &\leq \sum T_e(u) \cdot T_e(u) \leq \sum (p-1)^2 \\ \frac{p(p-1)}{2} \cdot \left(\frac{1}{p-1}\right)^2 &\leq PET(G) \leq \frac{p(p-1)}{2} \cdot (p-1)^2 \\ \frac{p}{2(p-1)} &\leq PET(G) \leq \frac{p(p-1)^3}{2} \end{aligned}$$

Result (ii) follows

2. Introduction to Octane Isomers

Octane possesses exactly 18 constitutional isomers. In mathematical chemistry, these molecules are modeled as connected, acyclic graphs (trees) denoted as $G = (V, E)$, where the vertex set represents the

carbon atoms ($|V| = 8$) and the edge set represents the carbon-carbon covalent bonds ($|E| = 7$). The hydrogen atoms are typically omitted in these hydrogen-depleted molecular graphs to focus purely on structural topology. For more details, we refer to [2],[6], [7] and [13]

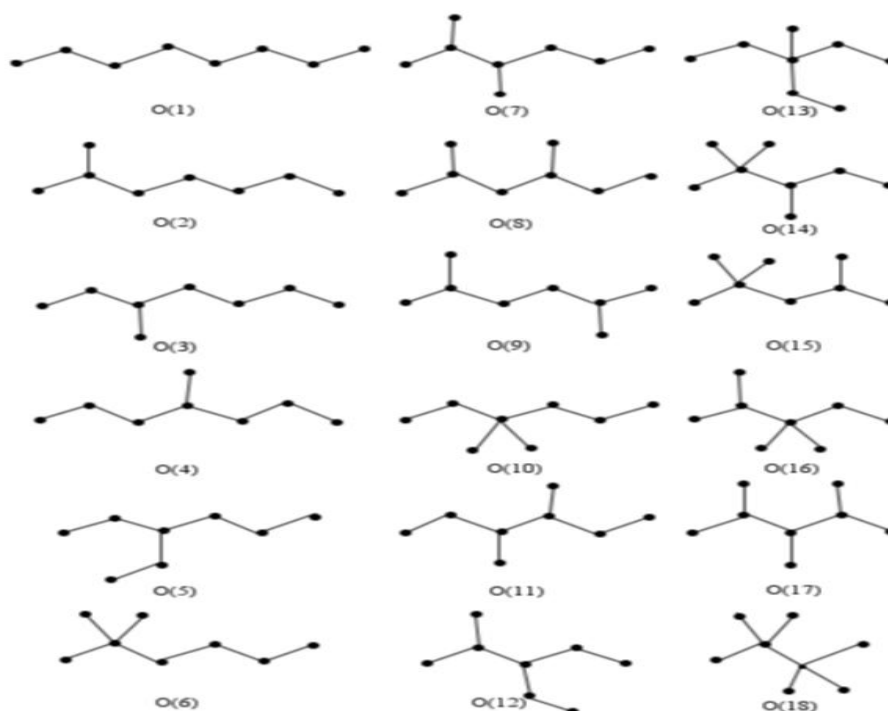


Figure 2.1: Molecular Graphs of Octane Isomers

Structural Profiles of the Octane Isomers

Isomer ID	IUPAC Name	Branching Type
O(1)	n-octane	Unbranched
O(2)	2-methylheptane	Mono-methyl
O(3)	3-methylheptane	Mono-methyl
O(4)	4-methylheptane	Mono-methyl
O(5)	3-ethylhexane	Mono-ethyl
O(6)	2,2-dimethylhexane	Di-methyl
O(7)	2,3-dimethylhexane	Di-methyl
O(8)	2,4-dimethylhexane	Di-methyl
O(9)	2,5-dimethylhexane	Di-methyl
O(10)	3,3-dimethylhexane	Di-methyl
O(11)	3,4-dimethylhexane	Di-methyl
O(12)	2-methyl-3-ethylpentane	Ethyl-methyl
O(13)	3-methyl-3-ethylpentane	Ethyl-methyl
O(14)	2,2,3-trimethylpentane	Tri-methyl

O(15)	2,2,4-trimethylpentane	Tri-methyl
O(16)	2,3,3-trimethylpentane	Tri-methyl
O(17)	2,3,4-trimethylpentane	Tri-methyl
O(18)	2,2,3,3-tetramethylbutane	Tetra-methyl

Eccentricity-Temperature indices of an octane isomers

Octane Isomers	SET(G)	PET(G)	DET(G)
O(1)	176.4	237.08	77.6
O(2)	104.524	94.159	32.8
O(3)	95.186	78.106	28.798
O(4)	90.524	70.161	29.464
O(5)	64.386	36.273	14.79
O(6)	69.048	41.7348	17.188
O(7)	56.924	28.245	13.992
O(8)	64.452	36.273	14.79
O(9)	69.048	41.73	15.456
O(10)	59.724	31.259	18.992
O(11)	59.724	31.259	12.792
O(12)	42.931	16.209	8.269
O(13)	40.131	14.1582	7.869
O(14)	42.931	16.2114	8.269
O(15)	45.731	18.4247	6.869
O(16)	40.131	14.1582	7.869
O(17)	42.931	16.6074	8.269
O(18)	29.862	6.5988	3.204

3. Graphical Representation of an Octane Isomers

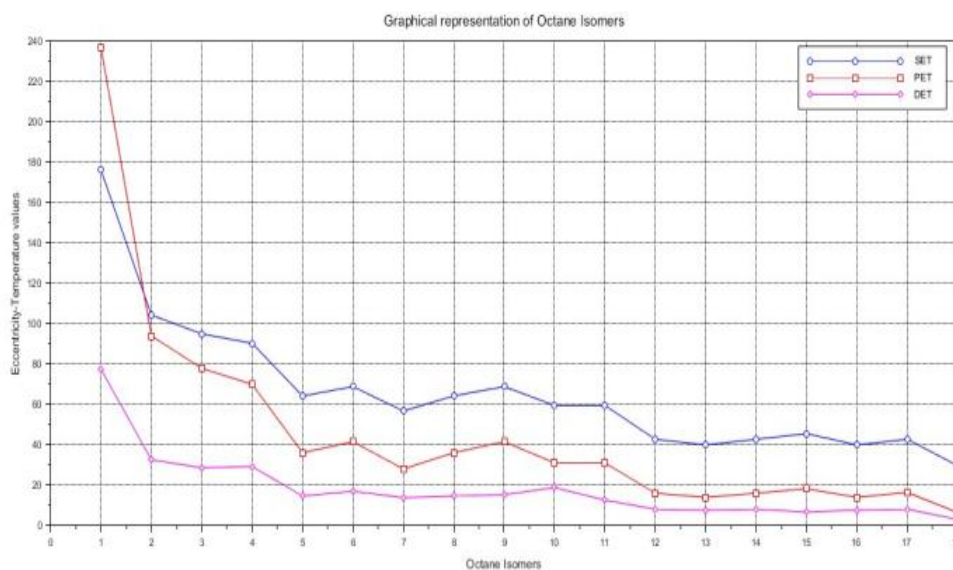


Figure 2. Graphical Representation of an Octane Isomers

The analytical plot maps the numerical values of three distinct eccentricity temperature based topological descriptors $SET(G)$, $PET(G)$, and $DET(G)$ against the structural domain of the 18 octane isomers along the horizontal axis x-axis.

In mathematical chemistry, these topological indices serve as structural descriptors optimized to map molecular shape parameters to macroscopic physicochemical properties, such as boiling point, acentric factor, and standard heat of vaporization.

The analytical plot maps the numerical values of three distinct eccentricity temperature based topological descriptors SET , PET , and DET against the structural domain of the 18 octane isomers along the horizontal axis x-axis.

In mathematical chemistry, these topological indices serve as structural descriptors optimized to map molecular shape parameters to macroscopic physicochemical properties, such as boiling point, acentric factor, and standard heat of vaporization.

Conclusions:

In this paper, we have studied eccentricity temperature based indices. We found exact values, bounds and characterisation of some graph families. which are not attempted it so far. This research raises a number of problems, including the following ones, about comparative advantages, applications, and mathematical properties viewpoint. Find the exact value of $SET(G)$, $PET(G)$ and $DET(G)$ of some chemical graphs / derived graphs / product graphs and explore some results towards QSPR / QSAR / QSTR model.

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Declaration of Competing Interest:

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper

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