

Behavior of Symmetric Deg Coindex and its Applications

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Abstract

In QSPR/QSAR investigations, topological indices, which are molecular graph invariants, are utilized to forecast the physicochemical characteristics of chemical compounds. In this research, we present the Symmetric deg coindex, a revolutionary degree-based topological index. Investigations into the topological index's mathematical features and a study of its link with various physicochemical aspects relating to lithium cluster and octane isomers were also conducted.

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MSC: 05C12, 05C76

1 Introduction

In studies of the quantitative structure-property relationship (QSPR) and the quantitative structure-activity relationship (QSAR), topological indices (TIs), often referred to as molecular descriptors, are crucial. By predicting the physico-chemical characteristics of compounds, they help to cut down on the amount of expensive and time-consuming investigations. In [5], the use of TIs in medication development and research was examined. Shanmukha et al. [12] recently looked into the QSPR analysis of TIs for anticancer medications and discovered that it had a high correlation with the physicochemical parameters. Numerous degree, distance, and eccentricity-based TIs have been investigated. The structure of the relevant molecular graph is specified to be a function of molecular descriptors [14,7,2]. Vukicevic et al. [13] demonstrated that these descriptors may be represented as the sum of edge contributions and dubbed them bond additive descriptors in their paper.

Let $\eta_{\mathcal{G}}(x)$ be the degree of a vertex x in \mathcal{G} . The following TIs are studied by various researchers;

- First Zagreb index and its coindex [7]: $M_1(\mathcal{G}) = \sum_{uv \in E(\mathcal{G})} (\eta_{\mathcal{G}}(u) + \eta_{\mathcal{G}}(v))$ and $\bar{M}_1(\mathcal{G}) = \sum_{uv \notin E(\mathcal{G})} (\eta_{\mathcal{G}}(u) + \eta_{\mathcal{G}}(v))$.
- F - index and its coindex [6,11]: $F(\mathcal{G}) = \sum_{uv \in E(\mathcal{G})} (\eta_{\mathcal{G}}^2(u) + \eta_{\mathcal{G}}^2(v))$ and $\bar{F}(\mathcal{G}) = \sum_{uv \notin E(\mathcal{G})} (\eta_{\mathcal{G}}^2(u) + \eta_{\mathcal{G}}^2(v))$.
- First modification Zagreb index [10]: $M_2^*(\mathcal{G}) = \sum_{uv \in E(\mathcal{G})} \frac{1}{\eta_{\mathcal{G}}(u)\eta_{\mathcal{G}}(v)}$.
- The redefined and hyper Zagreb coindices: $\overline{RZ}(\mathcal{G}) = \sum_{uv \notin E(\mathcal{G})} \frac{\eta_{\mathcal{G}}(u) + \eta_{\mathcal{G}}(v)}{\eta_{\mathcal{G}}(u)\eta_{\mathcal{G}}(v)}$ and $\overline{HZ}(\mathcal{G}) = \sum_{uv \notin E(\mathcal{G})} (\eta_{\mathcal{G}}(u) + \eta_{\mathcal{G}}(v))^2$.
- The second and third Zagreb coindices: $\bar{M}_2(\mathcal{G}) = \sum_{uv \in E(\mathcal{G})} \eta_{\mathcal{G}}(u)\eta_{\mathcal{G}}(v)$ and $\bar{M}_3(\mathcal{G}) = \sum_{uv \in E(\mathcal{G})} |\eta_{\mathcal{G}}(u) - \eta_{\mathcal{G}}(v)|$.

On the data sets of the IAMC, they examined a broad class of chemical descriptors known as discrete Adriatic TIs and discovered that twenty of them had substantial predictive characteristics. One among the useful Adriatic TIs is the symmetric deg (SD) index [13]

which is defined as $SD(\mathcal{G}) = \sum_{xy \in E(\mathcal{G})} \left(\frac{\eta_{\mathcal{G}}(x)}{\eta_{\mathcal{G}}(y)} + \frac{\eta_{\mathcal{G}}(y)}{\eta_{\mathcal{G}}(x)} \right)$. where $\eta_{\mathcal{G}}(x)$ is the degree of a

vertex x in \mathcal{G} . According to [13], SD invariant has been shown to have the best association with the total surface area of polychlorobiphenyls out of all the molecular descriptors currently in use. Motivated by the invariants like Zagreb and F -coindices, we propose

another invariant called symmetric deg coindex which is defined as $\overline{SD}(\mathcal{G}) = \sum_{uv \notin E(\mathcal{G})} \frac{\eta_{\mathcal{G}}(u)^2 + \eta_{\mathcal{G}}(v)^2}{\eta_{\mathcal{G}}(u)\eta_{\mathcal{G}}(v)}$.

2 Properties of \overline{SD}

We concentrate on certain bounds for the symmetric deg coindex of a particular connected graph in this section. A graph is referred to be a (s, e) graph if $|V| = s$ and $|E| = e$. A simple graph on the same set of \mathcal{G} vertices is the complement of \mathcal{G} , represented as $\bar{\mathcal{G}}$, where two vertices u and v are adjacent \Leftrightarrow they are not adjacent in \mathcal{G} .

Theorem 1. *Jensen's inequality [9]: For a convex function θ with an interval L and*

$$a_1, a_2, \dots, a_n \in L, \theta \left(\frac{a_1 + a_2 + \dots + a_n}{n} \right) \leq \frac{\theta(a_1) + \theta(a_2) + \dots + \theta(a_n)}{n}, \text{ with equality } \Leftrightarrow a_1 = a_2 = \dots = a_n.$$

Theorem 2. *If $\bar{\mathcal{G}}$ is a complement of \mathcal{G} , then*

$$4SD(\bar{G}) - SD(G) \leq 2(s-1)^2 M_2^*(G) - 2s(s-1) + \frac{2((s-1)^2 - 2\Delta + \Delta^2(s-1))}{(s-1)(s-1-2\delta)}$$

Proof. Note that the degree of a vertex v in G is $\eta_G(v)$. The degree of the same vertex in \bar{G} is given by $\eta_{\bar{G}}(v) = s - 1 - \eta_G(v)$. By the definition of SD index, we have

$$\begin{aligned} SD(\bar{G}) &= \sum_{xy \in E(\bar{G})} \left(\frac{\eta_{\bar{G}}^2(x) + \eta_{\bar{G}}^2(y)}{\eta_{\bar{G}}(x)\eta_{\bar{G}}(y)} \right) \\ &= \sum_{xy \in E(G)} \frac{(s-1-\eta_G(x))^2 + (s-1-\eta_G(y))^2}{(s-1-\eta_G(x))(s-1-\eta_G(y))} \\ &= \sum_{xy \in E(G)} \frac{(s-1)^2 + \eta_G^2(x) - 2(s-1)\eta_G(x) + (s-1)^2 + \eta_G^2(y) - 2(s-1)\eta_G(y)}{(s-1)^2 - (s-1)(\eta_G(x) + \eta_G(y)) + \eta_G(x)\eta_G(y)} \\ &= \sum_{xy \in E(G)} \frac{2(s-1)^2 - 2(s-1)(\eta_G(x) + \eta_G(y)) + (\eta_G^2(x) + \eta_G^2(y))}{(s-1)^2 - (s-1)(\eta_G(x) + \eta_G(y)) + \eta_G(x)\eta_G(y)}. \end{aligned}$$

By Jensen's inequality, we have

$$\begin{aligned} &\frac{1}{(s-1)(s-1 - (\eta_G(x) + \eta_G(y))) + \eta_G(x)\eta_G(y)} \\ &\leq \frac{1}{4(s-1)(s-1 - (\eta_G(x) + \eta_G(y)))} + \frac{1}{4\eta_G(x)\eta_G(y)} \end{aligned}$$

and equality holds $\Leftrightarrow (s-1)(s-1 - (\eta_G(x) + \eta_G(y))) = \eta_G(x)\eta_G(y)$.

Hence

$$\begin{aligned} SD(\bar{G}) &\leq \& \frac{1}{4} \sum_{xy \in E(G)} \left[2(s-1)^2 - 2(s-1)(\eta_G(x) + \eta_G(y)) + (\eta_G^2(x) + \eta_G^2(y)) \right] \\ &\quad \cdot \left(\frac{1}{(s-1)(s-1 - (\eta_G(x) + \eta_G(y)))} + \frac{1}{\eta_G(x)\eta_G(y)} \right) \\ &= \& \frac{1}{4} \sum_{xy \in E(G)} \left[\frac{2(s-1)^2}{(s-1)(s-1 - (\eta_G(x) + \eta_G(y)))} + \frac{2(s-1)^2}{\eta_G(x)\eta_G(y)} \right. \\ &\quad \left. - \frac{2(s-1)(\eta_G(x) + \eta_G(y))}{(s-1)(s-1 - (\eta_G(x) + \eta_G(y)))} - \frac{2(s-1)(\eta_G(x) + \eta_G(y))}{\eta_G(x)\eta_G(y)} \right] \end{aligned}$$

$$\begin{aligned}
 & \left. + \frac{\eta_G^2(x) + \eta_G^2(y)}{(s-1)(s-1-(\eta_G(x) + \eta_G(y)))} + \frac{\eta_G^2(x) + \eta_G^2(y)}{\eta_G(x)\eta_G(y)} \right] \\
 & \leq \& \frac{1}{4} \left[\frac{2(s-1)}{(s-1-2\delta)} + 2(s-1)^2 M_2^*(G) - \frac{4\delta}{(s-1-2\delta)} \right. \\
 & \quad \left. - 2(s-1)s + \frac{2\Delta^2}{(s-1)(s-1-2\delta)} + SD(G) \right] \\
 & = \& \frac{1}{4} \left[\frac{2(s-1)^2 - 4\Delta + 2\Delta^2(s-1)}{(s-1)(s-1-2\delta) - 2(s-1)s} + 2(s-1)^2 M_2^*(G) + SD(G) \right] \\
 \Rightarrow SD(\overline{G}) - \frac{SD(G)}{4} & \leq \& \frac{(s-1)^2}{2} M_2^*(G) - \frac{s(s-1)}{2} + \frac{(s-1)^2 - 2\Delta + \Delta^2(s-1)}{2(s-1)(s-1-2\delta)}
 \end{aligned}$$

Hence

$$4SD(\overline{G}) - SD(G) \leq 2(s-1)^2 M_2^*(G) - 2s(s-1) + \frac{2((s-1)^2 - 2\Delta + \Delta^2(s-1))}{(s-1)(s-1-2\delta)}.$$

□

Theorem 3. Let G be a (s, e) -graph with maximal degree Δ . Then $\overline{SD}(G) \leq \frac{1}{\delta^2} [(s-1)M_1(G) - F(G) + s(s-1)\Delta^2 - 2e\Delta^2]$.

Proof. Let $xy \in E(G)$. Then $s-1-\eta_G(x)$ vertices are non-adjacent with the vertex x in $V(G)$. For $xz \notin E(G)$,

$$\begin{aligned}
 \eta_G^2(x) + \eta_G^2(z) & \leq (\eta_G^2(x) + \Delta^2)(s-1-\eta_G(x)) \\
 & = (s-1)\eta_G^2(x) - \eta_G^3(x) + (s-1)\Delta^2 - \Delta^2\eta_G(x)
 \end{aligned}$$

By the definition of \overline{SD} , we have

$$\begin{aligned}
 & = \sum_{xz \notin E(G)} \frac{\eta_G^2(x) + \eta_G^2(z)}{\eta_G(x)\eta_G(y)} \\
 & \leq \frac{1}{\delta^2} \sum_{x \in V(G)} [(s-1)\eta_G^2(x) - \eta_G^3(x) + (s-1)\Delta^2 - \Delta^2\eta_G(x)] \\
 & = \frac{1}{\delta^2} [(s-1)M_1(G) - F(G) + s(s-1)\Delta^2 - 2e\Delta^2] \quad \square
 \end{aligned}$$

Theorem 4. Let \mathcal{G} be a (s, e) -graph with t pendent vertices.

Then $\overline{SD}(\mathcal{G}) \geq \frac{5st}{2} - \frac{3t^2}{2} - \frac{7t}{2}$ and equality holds $\Leftrightarrow \mathcal{G} \cong P_s$.

Proof. Assume that the graph \mathcal{G} has exactly one pendent vertex, say x , and that y is the unique neighbour of x .

Then

$$\overline{SD}(\mathcal{G}) \geq \sum_{z \in V(\mathcal{G}) \setminus \{x,y\}} \left(\frac{1 + \eta_{\mathcal{G}}^2(w)}{\eta_{\mathcal{G}}(w)} \right)_{z \in V(\mathcal{G}) \setminus \{x,y\}} \binom{5}{2} = \frac{5(s-2)}{2}.$$

Let $t \geq 2$. Each pair of pendent vertices contribute 2 to $\overline{SD}(\mathcal{G})$. Thus the total contribution of pendent vertices pairs to $\overline{SD}(\mathcal{G})$ is $2\binom{t}{2} = t(t-1)$.

Let x be a pendent vertex in \mathcal{G} and let y be its unique neighbor. If $z \in V(\mathcal{G})$ is any non pendent vertex other than x and y , the contribution of vertex pairs $\{x, z\}$ to $\overline{SD}(\mathcal{G})$ is $\frac{1 + \eta_{\mathcal{G}}^2(w)}{\eta_{\mathcal{G}}(w)}$. The total contribution of such vertex pairs $\{x, z\}$ to $\overline{SD}(\mathcal{G})$ are $(s-t-1)t \left(\frac{1 + \eta_{\mathcal{G}}^2(w)}{\eta_{\mathcal{G}}(w)} \right)$.

Since $\eta_{\mathcal{G}}(z) \geq 2$ for non-pendent vertex z in G , we get

$$\begin{aligned} \overline{SD}(\mathcal{G}) &\geq t(t-1) + t(s-t-1) \binom{5}{2} \\ &= \frac{5st}{2} - \frac{3t^2}{2} - \frac{7t}{2}. \end{aligned}$$

Equality holds $\Leftrightarrow \mathcal{G} \cong P_s$, where P_s is a path on s vertices. □

Theorem 5. Let \mathcal{G} be a (s, e) -graph with t pendent vertices and maximum degree Δ . If δ_1 is a non-pendent minimum degree, then $\alpha \leq \overline{SD}(\mathcal{G}) \leq \beta$, where

$$\begin{aligned} \alpha &= t(t-1) \left(\frac{\Delta^2 - \delta_1^2}{\Delta^2} \right) + t(s-t-1) \frac{\Delta(1 + \delta_1^2) - 2\delta_1^2}{\Delta^2} + \frac{(s(s-1) - 2e)\delta_1^2}{\Delta^2} \\ \beta &= t(t-1) \left(\frac{\delta_1^2 - \Delta^2}{\delta_1^2} \right) + t(s-t-1) \left(\frac{\delta_1(1 + \Delta^2) - 2\Delta^2}{\delta_1^2} \right) + \frac{(s(s-1) - 2e)\Delta^2}{\delta_1^2}. \end{aligned}$$

Equality holds $\Leftrightarrow \mathcal{G}$ is a regular graph.

Proof. One can see that the number of vertex pairs (x, y) such that $xy \notin E(\mathcal{G})$ is $\frac{s(s-1)}{2} - e$. Since the number of pendent vertices in a connected graph \mathcal{G} is t , we have the following:

- (i) Number of vertex pairs (x, y) such that $xy \notin E(G)$ with $\eta_G(x) = \eta_G(y) = 1$ is $\frac{t(t-1)}{2}$.
- (ii) Number of vertex pairs (x, y) such that $xy \notin E(G)$ with $\eta_G(x) = 1$ or $\eta_G(y) = 1$ is $t(s - t - 1)$.
- (iii) Number of vertex pairs (x, y) such that $xy \notin E(G)$ with $\eta_G(x) > 1$ and $\eta_G(y) > 1$ is $\frac{s(s-1)}{2} - e - \frac{t(t-1)}{2} - t(s - t - 1)$.

Therefore

$$\begin{aligned} \overline{SD}(G) &= \sum_{\substack{xy \notin E(G) \\ \eta_G(x)=\eta_G(y)=1}} \frac{\eta_G^2(x) + \eta_G^2(y)}{\eta_G(x)\eta_G(y)} + \sum_{\substack{xy \notin E(G) \\ \eta_G(x)=1, \eta_G(y)>1}} \frac{\eta_G^2(x) + \eta_G^2(y)}{\eta_G(x)\eta_G(y)} \\ &\quad + \sum_{xy \notin E(G), \eta_G(x), \eta_G(y) > 1} \frac{\eta_G^2(x) + \eta_G^2(y)}{\eta_G(x)\eta_G(y)} \\ &\geq \frac{t(t-1)}{2} (2) + t(s-t-1) \left(\frac{1 + \delta_1^2}{\Delta} \right) + \frac{2\delta_1^2}{\Delta^2} \left(\frac{s(s-1)}{2} - e - \frac{t(t-1)}{2} - t(s-t-1) \right) \\ &= t(t-1) \left(\frac{\Delta^2 - \delta_1^2}{\Delta^2} \right) + \frac{t(s-t-1)}{\Delta^2} (\Delta(1 + \delta_1^2) - 2\delta_1^2) + \frac{s(s-1)\delta_1^2}{\Delta^2} - \frac{2\delta_1^2 e}{\Delta^2} \end{aligned}$$

Equality holds $\Leftrightarrow \delta_1 = \Delta$, this implies, G is a regular graph.

Analogously above case, we obtain

$$\begin{aligned} \overline{SD}(G) &\leq t(t-1) + t(s-t-1) \left(\frac{1 + \Delta^2}{\delta_1} \right) + \frac{2\Delta^2}{\delta_1^2} \left(\frac{s(s-1)}{2} - e - \frac{t(t-1)}{2} - t(s-t-1) \right) \\ &= t(t-1) \left(\frac{\delta_1^2 - \Delta^2}{\delta_1^2} \right) + t(s-t-1) \left(\frac{\delta_1(1 + \Delta^2) - 2\Delta^2}{\delta_1^2} \right) + \frac{s(s-1)\Delta^2}{\delta_1^2} - \frac{2\Delta^2 e}{\delta_1^2} \end{aligned}$$

with equality $\Leftrightarrow \delta_1 = \Delta$. This implies G is regular. □

Setting $t = 0$ in the above theorem, we obtain the following corollary.

Corollary 1. Let G be a (s, e) -graph with non-pendent minimum degree δ_1 . Then

$$\frac{(s(s-1)-2e)\delta_1^2}{\Delta^2} \leq \overline{SD}(G) \leq \frac{(s(s-1)-2e)\Delta}{\delta_1^2} \text{ with equality } \Leftrightarrow G \text{ is regular.}$$

Theorem 6. Let G be a (s, e) -graph with t pendent vertices. Then $\alpha \leq \overline{SD}(G) \leq \beta$, where

$$\alpha = \frac{t(t-1)(2\Delta\delta - \Delta^2 - \delta^2)}{2\Delta\delta} + t(s-t-1) \left(\delta + \frac{1}{\delta} - \frac{\delta}{\Delta} - \frac{\Delta}{\delta} \right) + \frac{(s(s-1) - 2e)(\Delta^2 + \delta^2)}{2\Delta\delta}$$

and

$$\beta = \frac{t(t-1)(2\delta\Delta - \Delta^2 - \delta^2)}{2\Delta\delta} + t(s-t-1) \left(\Delta + \frac{1}{\Delta} - \frac{\Delta}{\delta} - \frac{\delta}{\Delta} \right) + \frac{(s(s-1) - 2e)(\Delta^2 + \delta^2)}{2\delta\Delta}.$$

Proof. If $xy \notin E(G)$ with $\eta_G(x) > 1$ and $\eta_G(y) > 1$, then

$$\left(\frac{\delta}{\Delta} + \frac{\Delta}{\delta} \right) \leq \frac{\eta_G(x)}{\eta_G(y)} + \frac{\eta_G(y)}{\eta_G(x)} \leq \left(\frac{\Delta}{\delta} + \frac{\delta}{\Delta} \right)$$

Similarly for non adjacent vertices x and y in G with $\eta_G(x) > 1$ and $\eta_G(y) = 1$. We have

$$\delta + \frac{1}{\delta} \leq \frac{\eta_G(x)}{\eta_G(y)} + \frac{\eta_G(y)}{\eta_G(x)} \leq \Delta + \frac{1}{\Delta}$$

One can easily observe that for each $xy \in E(G)$ with $\eta_G(x), \eta_G(y) \leq s - 2$.

$$\begin{aligned} \overline{SD}(G) &= \sum_{\substack{xy \in E(G) \\ \eta_G(x), \eta_G(y) = 1}} \left(\frac{\eta_G(x)}{\eta_G(y)} + \frac{\eta_G(y)}{\eta_G(x)} \right) + \sum_{\substack{xy \in E(G) \\ \eta_G(x) > 1, \eta_G(y) = 1}} \left(\frac{\eta_G(x)}{\eta_G(y)} + \frac{\eta_G(y)}{\eta_G(x)} \right) \\ &\quad + \sum_{xy \in E(G) \eta_G(x) > 1, \eta_G(y) > 1} \left(\frac{\eta_G(x)}{\eta_G(y)} + \frac{\eta_G(y)}{\eta_G(x)} \right) \\ &\geq \sum_{\substack{xy \in E(G) \\ \eta_G(x), \eta_G(y) = 1}} (2) + \sum_{xy \in E(G) \eta_G(x) > 1, \eta_G(y) = 1} \left(\delta + \frac{1}{\delta} \right) + \sum_{xy \in E(G) \eta_G(x) > 1, \eta_G(y) > 1} \left(\frac{\delta}{\Delta} + \frac{\Delta}{\delta} \right) \\ &= \frac{2t(t-1)}{2} + \left(\delta + \frac{1}{\delta} \right) (s-t-1)t + \left(\frac{\delta}{\Delta} + \frac{\Delta}{\delta} \right) \left(\frac{s(s-1)}{2} - e - \frac{t(t-1)}{2} - t(s-t-1) \right) \\ &= \frac{t(t-1)(2\Delta\delta - \Delta^2 - \delta^2)}{2\Delta\delta} + t(s-t-1) \left(\delta + \frac{1}{\delta} - \frac{\Delta}{\delta} - \frac{\delta}{\Delta} \right) + \frac{(s(s-1) - 2e)(\Delta^2 + \delta^2)}{2\delta\Delta}. \end{aligned}$$

Hence

Similarly we obtain the upper bound.

$$\begin{aligned} \overline{SD}(G) &\leq \frac{2t(t-1)}{2} + \left(\Delta + \frac{1}{\Delta} \right) (s-t-1)t + \left(\frac{\Delta}{\delta} + \frac{\delta}{\Delta} \right) \left(\frac{s(s-1)}{2} - e - \frac{t(t-1)}{2} - t(s-t-1) \right) \\ &= \frac{t(t-1)(2\delta\Delta - \Delta^2 - \delta^2)}{2\Delta\delta} + t(s-t-1) \left(\Delta + \frac{1}{\Delta} - \frac{\Delta}{\delta} - \frac{\delta}{\Delta} \right) + \frac{(s(s-1) - 2e)(\Delta^2 + \delta^2)}{2\delta\Delta}. \end{aligned}$$

□

Setting $t = 0$ in the above theorem, we get the following corollary.

Corollary 2. Let \mathcal{G} be a (s, e) -graph with no pendent vertices. Then

$$\frac{(s(s - 1) - 2e)(\Delta^2 + \delta^2)}{2\delta\Delta} \leq \overline{SD}(\mathcal{G}) \leq \frac{(s(s - 1) - 2e)(\Delta^2 + \delta^2)}{2\delta\Delta}.$$

Theorem 7. Let \mathcal{G} be graph with s vertices. Then $\frac{\overline{F}(\mathcal{G})}{(s-2)^2} \leq \overline{SD}(\mathcal{G}) \leq \overline{F}(\mathcal{G})$

Proof. Note that for each edge $xy \notin E(\mathcal{G})$, $\eta_{\mathcal{G}}(x), \eta_{\mathcal{G}}(y) \leq s - 2$. Hence by the definition of \overline{SD} and above fact, we have

$$\overline{SD}(\mathcal{G}) = \sum_{xy \notin E(\mathcal{G})} \frac{\eta_{\mathcal{G}}^2(x) + \eta_{\mathcal{G}}^2(y)}{\eta_{\mathcal{G}}(x)\eta_{\mathcal{G}}(y)} \geq \sum_{xy \notin E(\mathcal{G})} \frac{\eta_{\mathcal{G}}^2(x) + \eta_{\mathcal{G}}^2(y)}{(s - 2)^2} = \frac{\overline{F}(\mathcal{G})}{(s - 2)^2}.$$

Similarly, we prove

$$\overline{SD}(\mathcal{G}) = \sum_{xy \notin E(\mathcal{G})} \frac{\eta_{\mathcal{G}}^2(x) + \eta_{\mathcal{G}}^2(y)}{\eta_{\mathcal{G}}(x)\eta_{\mathcal{G}}(y)} \leq \sum_{xy \notin E(\mathcal{G})} (\eta_{\mathcal{G}}^2(x) + \eta_{\mathcal{G}}^2(y)) = \overline{F}(\mathcal{G}). \quad \square$$

Theorem 8. Let \mathcal{G} be a (s, e) -graph. Then

$$\overline{SD}(\mathcal{G}) \geq \left(\frac{2}{s - 2}\right) \overline{M}_1(\mathcal{G}) - s(s - 1) + 2e$$

Proof.

$$\begin{aligned} \overline{SD}(\mathcal{G}) &= \sum_{xy \notin E(\mathcal{G})} \left(\frac{\eta_{\mathcal{G}}(x)}{\eta_{\mathcal{G}}(y)} + \frac{\eta_{\mathcal{G}}(y)}{\eta_{\mathcal{G}}(x)} \right) \\ &= \sum_{xy \notin E(\mathcal{G})} \left(\left(\frac{1}{\eta_{\mathcal{G}}(x)} + \frac{1}{\eta_{\mathcal{G}}(y)} \right) (\eta_{\mathcal{G}}(x) + \eta_{\mathcal{G}}(y)) - 2 \right). \end{aligned}$$

For each pair of vertices x and y not in $E(\mathcal{G})$ in \mathcal{G} , $\eta_{\mathcal{G}}(x) \leq s - 2$ and $\eta_{\mathcal{G}}(y) \leq s - 2$. Hence

$$\begin{aligned} \overline{SD}(\mathcal{G}) &\geq \frac{2}{s - 2} \sum_{xy \notin E(\mathcal{G})} (\eta_{\mathcal{G}}(x) + \eta_{\mathcal{G}}(y)) - 2 \left(\frac{s(s - 1)}{2} - e \right) \\ &= \frac{2}{s - 2} \overline{M}_1(\mathcal{G}) - s(s - 1) + 2e. \end{aligned}$$

□

Theorem 9. Let \mathcal{G} be a (s, e) -graph. Then

$$\overline{SD}(\mathcal{G}) \leq 2(s - 2)\overline{RZ}(\mathcal{G}) - s(s - 1) + 2e.$$

Proof.

$$\begin{aligned} \overline{SD}(\mathcal{G}) &= \sum_{xy \notin E(\mathcal{G})} \left(\frac{\eta_{\mathcal{G}}(x)}{\eta_{\mathcal{G}}(y)} + \frac{\eta_{\mathcal{G}}(y)}{\eta_{\mathcal{G}}(x)} \right) \\ &= \sum_{xy \notin E(\mathcal{G})} \left(\left(\frac{1}{\eta_{\mathcal{G}}(x)} + \frac{1}{\eta_{\mathcal{G}}(y)} \right) (\eta_{\mathcal{G}}(x) + \eta_{\mathcal{G}}(y) - 2) \right). \end{aligned}$$

It is clear that for each $xy \notin E(\mathcal{G}), \eta_{\mathcal{G}}(x), d(y) \leq a - 2$. Hence

$$\begin{aligned} \overline{SD}(\mathcal{G}) &\leq 2(s - 2) \sum_{xy \notin E(\mathcal{G})} \frac{\eta_{\mathcal{G}}(x) + \eta_{\mathcal{G}}(y)}{\eta_{\mathcal{G}}(x)\eta_{\mathcal{G}}(y)} - 2 \left(\frac{s(s - 1)}{2} \right) + 2e \\ &= 2(s - 2)\overline{RZ}(\mathcal{G}) - s(s - 1) + 2e. \end{aligned}$$

Equality holds $\Leftrightarrow \eta_{\mathcal{G}}(x) = \eta_{\mathcal{G}}(y) = s - 2, \forall xy \notin E(\mathcal{G})$. This implies each vertex of \mathcal{G} has degree $s - 1$ or $s - 2$. Thus $\mathcal{G} \cong K_n$ (or) $(s - 2)$ -regular (or) $(s - 1, s - 2)$ -regular. \square

Theorem 10. Let \mathcal{G} be a (s, e) -graph. Then

$$\frac{(\overline{M}_3(\mathcal{G}))^2}{e(s - 2)^2} + \frac{2\overline{M}_2(\mathcal{G})}{(s - 2)^2} \leq \overline{SD}(\mathcal{G}) \leq \overline{HZ}(\mathcal{G}) - 2\overline{M}_2(\mathcal{G}).$$

Equality holds $\Leftrightarrow |d(x) - d(y)| = c, \forall xy \notin E(\mathcal{G})$.

Proof.

$$\begin{aligned} \overline{SD}(\mathcal{G}) &\leq \sum_{xy \notin E(\mathcal{G})} (\eta_{\mathcal{G}}^2(x) + \eta_{\mathcal{G}}^2(y)) \\ &= \sum_{xy \notin E(\mathcal{G})} \left((\eta_{\mathcal{G}}(x) + \eta_{\mathcal{G}}(y))^2 - 2\eta_{\mathcal{G}}(x)\eta_{\mathcal{G}}(y) \right) \\ &= \overline{HZ}(\mathcal{G}) - 2\overline{M}_2(\mathcal{G}) \\ \overline{SD}(\mathcal{G}) &\geq \frac{1}{(s - 2)^2} \left(\sum_{xy \notin E(\mathcal{G})} (\eta_{\mathcal{G}}^2(x) - 2\eta_{\mathcal{G}}(x)\eta_{\mathcal{G}}(y) + \eta_{\mathcal{G}}^2(y)) + 2 \sum_{xy \notin E(\mathcal{G})} \eta_{\mathcal{G}}(x)\eta_{\mathcal{G}}(y) \right) \\ &= \frac{1}{(s - 2)^2} \left(\sum_{xy \notin E(\mathcal{G})} |\eta_{\mathcal{G}}(x) - \eta_{\mathcal{G}}(y)|^2 + 2\overline{M}_2(\mathcal{G}) \right) \end{aligned}$$

By Cauchy's -Schwarz inequality, we have

$$\begin{aligned}\overline{SD}(G) &\geq \frac{1}{b(a-2)^2} \sum_{xy \notin E(G)} |\eta_G(x) - \eta_G(y)|^2 + \frac{2}{(s-2)^2} \overline{M}_2(G) \\ &= \frac{1}{e(s-2)^2} \overline{M}_3(G)^2 + \frac{2}{(s-2)^2} \overline{M}_2(G)\end{aligned}$$

Equality holds $\Leftrightarrow |d(x) - d(y)| = c$, where c is a constant $\forall xy \notin E(G)$. □

3 QSPR analysis for Symmetric deg coindex \overline{SD}

In this section, we investigate the correlation of some chemical properties of octane isomers and Li_n clusters with \overline{SD} descriptor.

3.1 Regression model for octane isomers

The molecular graphs of octane isomers are shown in Figure 1 as per the order of our calculation. The experimental values of physico-chemical properties of octane isomers shown in Table 1 are taken from the free online resource - Milano Chemometrics and QSAR Research Group (<http://www.moleculardescriptors.eu/dataset/dataset.htm>).

We have tested the following linear regression models

$$P = m(TD) + C, \tag{1}$$

where P is the physical property of the octane isomer and TD is the topological descriptor.

Using the above formula we have the following linear regression models for \overline{SD} .

$$\text{Boiling point (BP)} = (-1.1976)\overline{SD} + 166.1942$$

$$\text{Melting point (MP)} = (57.0379)\overline{SD} - 2580.7737$$

$$\text{Heat capacity (CT)} = (-1.16742)\overline{SD} + 363.0505$$

$$\text{Entropy (S)} = (-0.070547)\overline{SD} + 136.3352$$

$$\text{Density (DENS)} = (0.00082)\overline{SD} + 0.67964$$

$$\text{(HFORM)} = (-0.31213)\overline{SD} - 38.15059$$

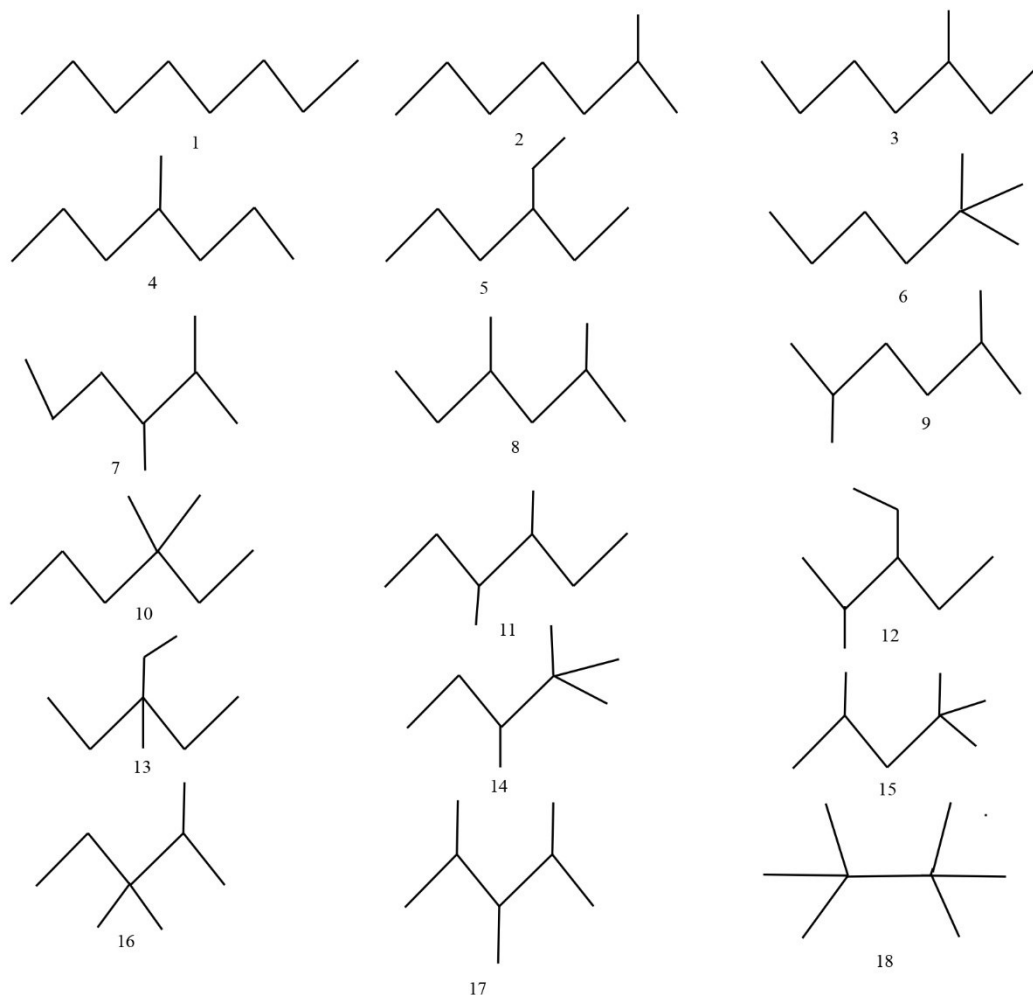


Figure:1 Molecular graphs of Octane isomers.

Chemical property	Correlation coefficient	Coefficient of determination	Standard error of estimate
Boiling point	-0.3795	0.155977604	5.8335
Melting point	0.217799	0.047436404	510.6913
Heat capacity	0.333255	0.111058895	9.4639
Entropy	-0.302695	0.091624263	4.4381
Density	0.054324	0.002951097	0.030091
HFORM	-0.483438	0.2337123	1.129235

Table 1: Chemical properties and \overline{SD} of Octane isomers

Molecule	BP	MP	CT	S	DENS	HFORM	\overline{SD}
n-octane	125.665	216.3	296.2	111.67	0.7025	-49.82	42.3333
2-methyl-heptane	117.647	164.16	288	109.84	0.698	-51.5	42.6833
3-methyl-heptane	118.925	152.6	292	111.26	0.7058	-50.82	42.7667
4-methyl-heptane	117.709	152	290	109.32	0.7046	-50.69	42.7667
3-ethyl-hexane	118.534	-999	292	109.43	0.7136	-50.4	42.85
2,2-dimethyl-hexane	106.84	151.97	279	103.42	0.6953	-53.71	43.4
2,3-dimethyl-hexane	115.607	-999	293	108.02	0.7121	-51.13	43.2167
2,4-dimethyl-hexane	109.429	-999	282	106.98	0.7004	-52.44	43.1167
2,5-dimethyl-hexane	109.103	182	279	105.72	0.6935	-53.21	51.1667
3,3-dimethyl-hexane	111.969	147	290.84	104.74	0.71	-52.61	43.6
3,4-dimethyl-hexane	117.725	-999	298	106.59	0.72	-50.91	43.3
2-methyl-3-ethyl-pentane	115.45	158.2	295	106.06	0.7193	-50.48	43.3
3-methyl-3-ethyl-pentane	118.259	182.2	305	101.48	0.7274	-51.38	43.8
2,2,3-trimethyl-pentane	109.841	160.89	294	101.31	0.7161	-52.61	44.0667
2,2,4-trimethyl-pentane	99.238	165.8	271.15	104.09	0.6919	-53.57	43.75
2,3,3-trimethyl-pentane	114.76	172.22	303	102.06	0.7262	-51.73	44.1833
2,3,4-trimethyl-pentane	113.467	163.9	295	102.39	0.7191	-51.97	43.6667
2,2,3,3-tetramethylbutane	106.47	373.8	270.8	93.06	0.8242	-53.99	45

Table 2: Correlation analysis of physical properties of octane isomers and \overline{SD}

The following scatter plots show the relationship between the chemical characteristics and \overline{SD} index of the octane isomers using the data from Table 1. We note a correlation between the physical characteristics of octane isomers and the \overline{SD} index. Figures 2 to 7 show the relationship between \overline{SD} and several physio-chemical characteristics. Table 2 compares the \overline{SD} description with the physio-chemical characteristics of octane isomers.

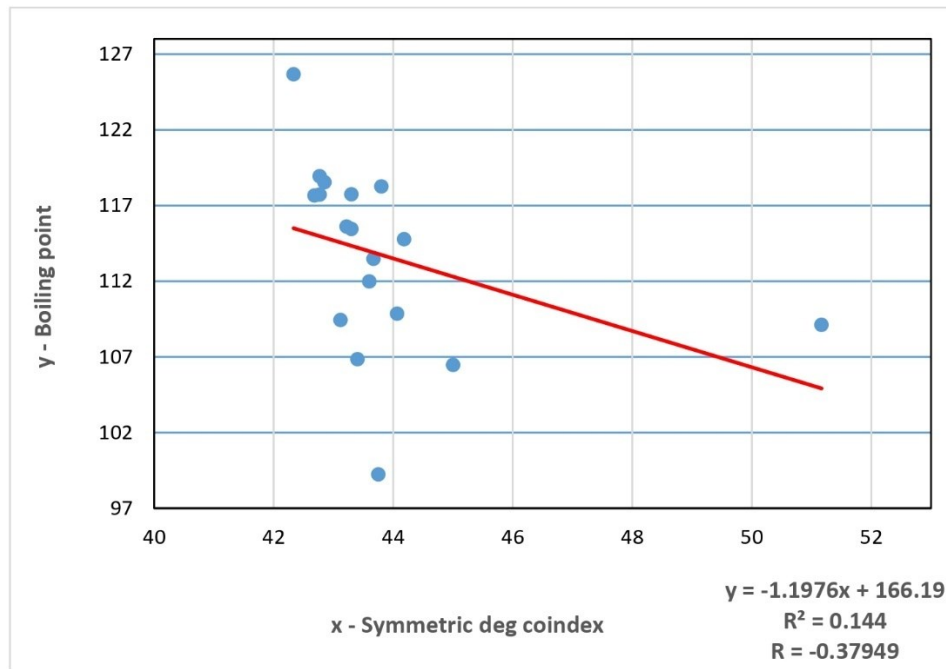


Figure:2 Scatter plot between boiling point and \overline{SD} descriptor of octane isomers

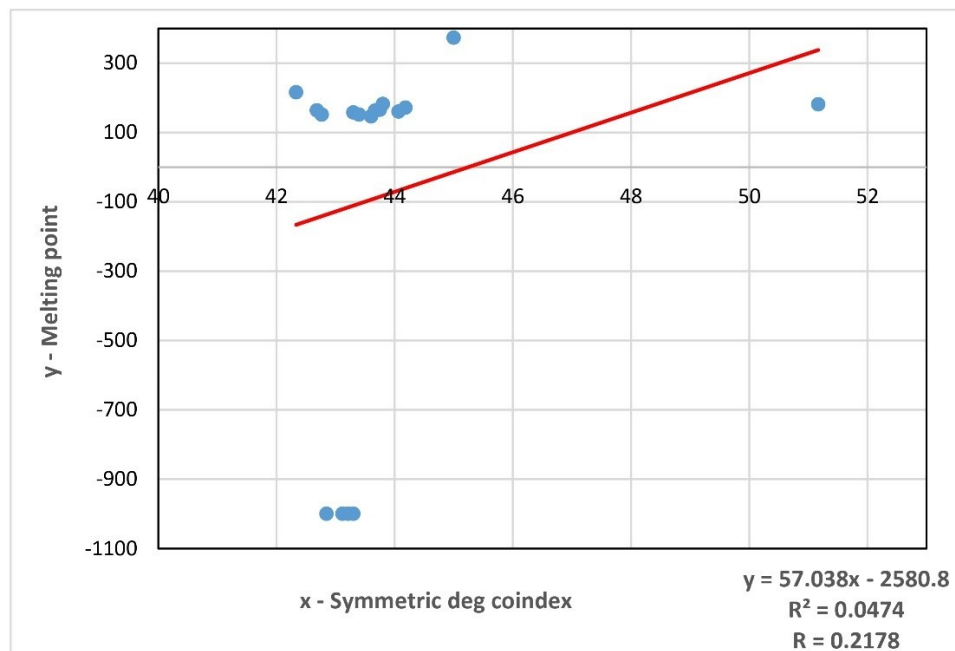


Figure:3 Scatter plot between melting point and \overline{SD} descriptor of octane isomers

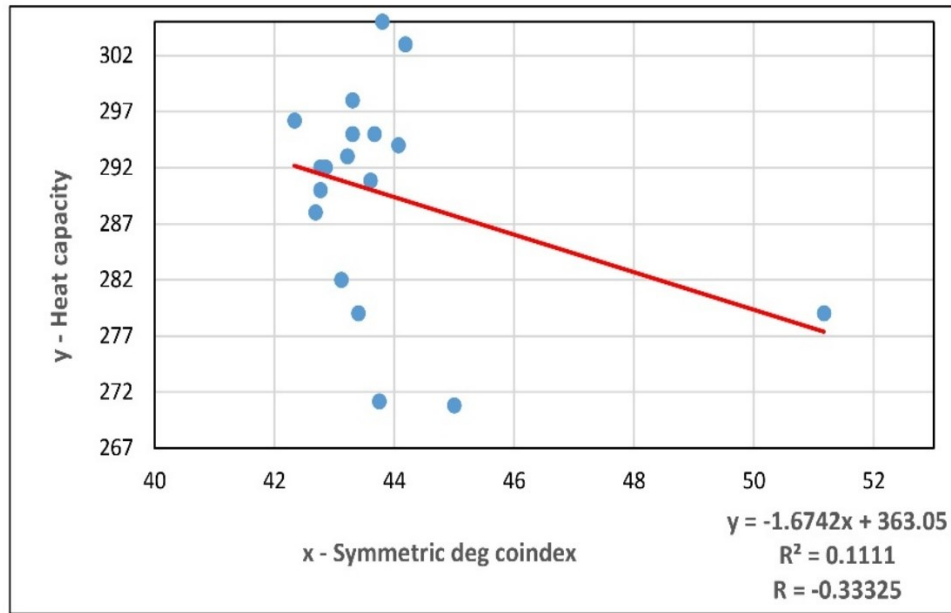


Figure:4 Scatter plot between heat capacity and \overline{SD} descriptor of octane isomers

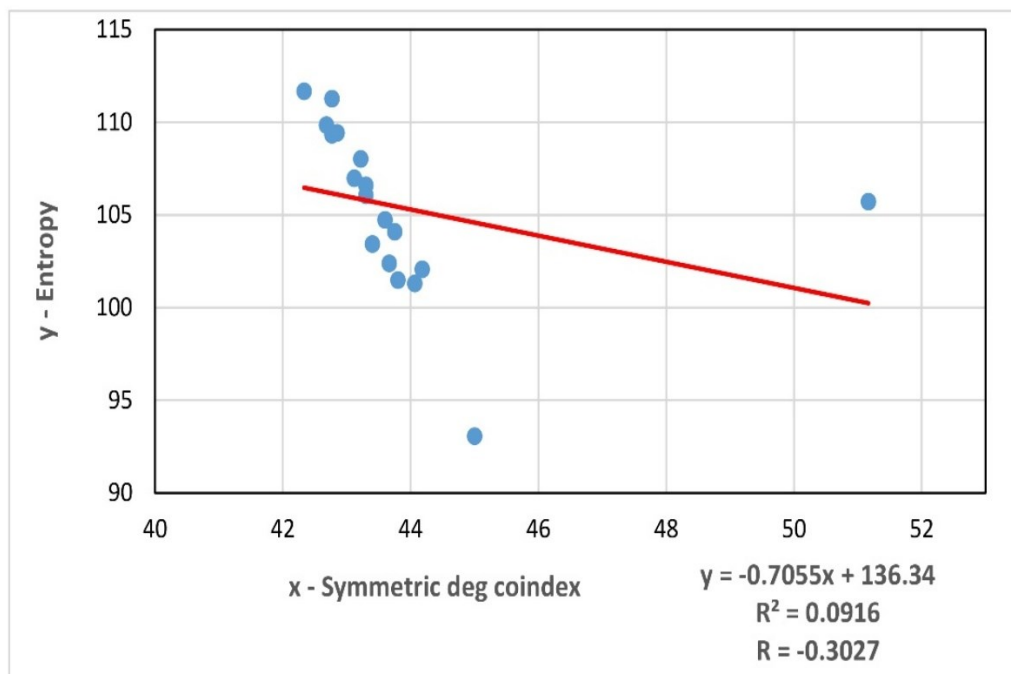


Figure:5 Scatter plot between entropy and \overline{SD} descriptor of octane isomers

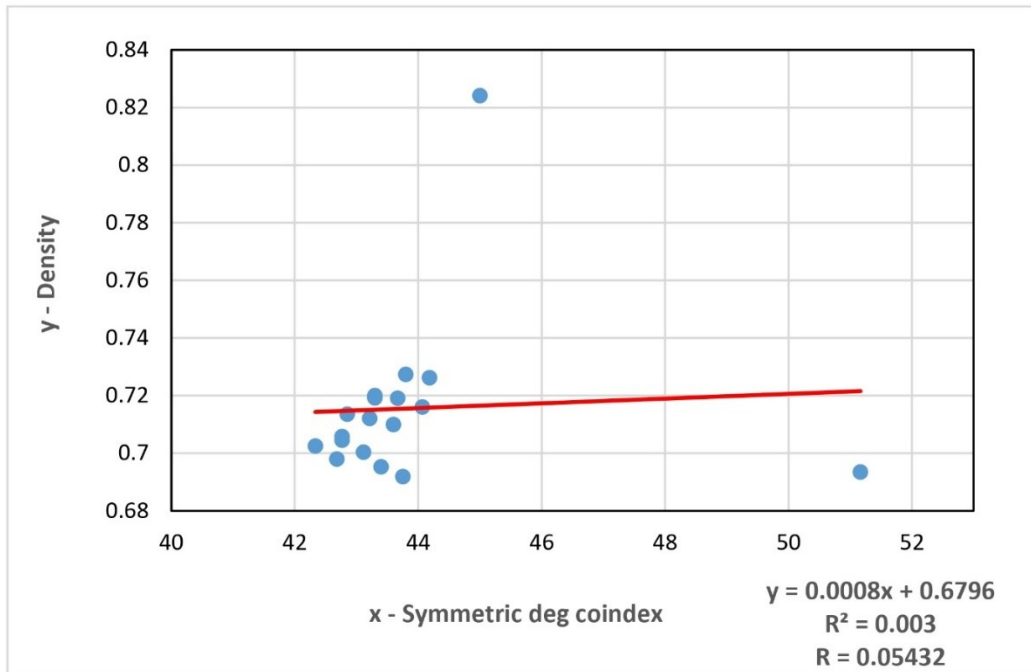


Figure:6 Scatter plot between density and \overline{SD} descriptor of octane isomers

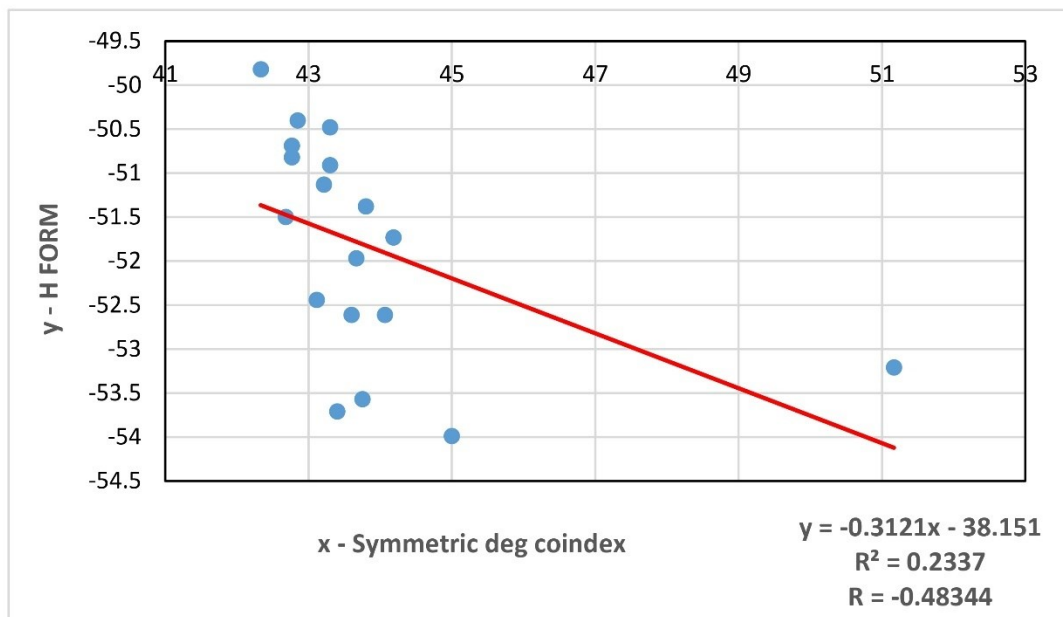


Figure:7 Scatter plot between HFORM and \overline{SD} descriptor of octane isomers

3.2 Regression model for Li_n cluster

Minimized structures obtained for Li_n clusters ($n = 2$ to 10) using DFT-based DMol³ program were considered for constructing the molecular graph (see Figure 8). Based on these structures, we worked on the symmetric deg coindex descriptor such that each structure corresponds to a real number.

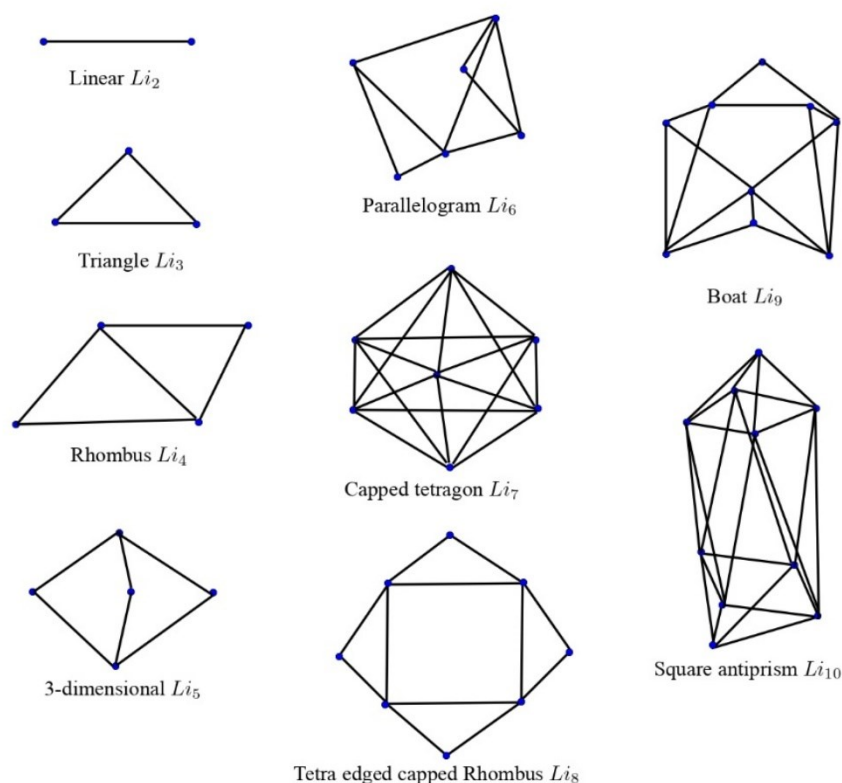


Figure:8 Molecular graph of Li_n cluster. Blue dots represent Li atom.

We have the linear regression model

$$P = m(TD) + C, \quad (2)$$

where P is the physical property of the Li_n clusters and TD is the topological descriptor.

Now we establish the relation using equation (2) between \overline{SD} with binding energy per atom and average bond length and total energy of Li_n clusters using Table 3.

From Equation (2), we have the following linear model for chemical properties of Li_n cluster and Symmetric deg coindex \overline{SD} .

$$\begin{aligned} \text{Binding energy (eV/ atom)} &= (0.00743)\overline{SD} + 0.61445 \\ \text{Average bond length (\AA)} &= (-0.0222)\overline{SD} + 2.49601 \\ \text{Total energy (eV)} &= (-28.09265)\overline{SD} - 754.41732 \end{aligned}$$

$Li_n (n = 2 \text{ to } 10)$	Binding energy (eV/atom)	Average bond length (\AA)	Total energy (eV)	\overline{SD}
Li_2	0.46	2.7	-407.9149	
Li_3	0.48	2.92	-611.92252	
Li_4	0.66	2.34	-816.62403	2
Li_5	0.72	2.42	-1021.04142	8
Li_6	0.8	1.85	-1225.73325	15
Li_7	0.86	1.87	-1430.44691	6
Li_8	0.88	1.83	-1635.01045	34.1333
Li_9	0.89	1.69	-1839.42875	41.53333
Li_{10}	0.91	1.49	-2043.98649	44.4

Table 3: Molecular graph $Li_n (n = 2 \text{ to } 10)$ and its Binding energy per atom (eV), Average bond length (A) and Total energy (eV)

The following scatter plots are made between the chemical characteristics and the \overline{SD} index of the molecular graph of lithium using the information from Table 3. We note a correlation between the L in cluster's attributes and the \overline{SD} index. Figures 9 to 11 show how \overline{SD} correlates with several physio-chemical characteristics. Table4 compares the physio-chemical characteristics of the lithium cluster with those of the \overline{SD} .

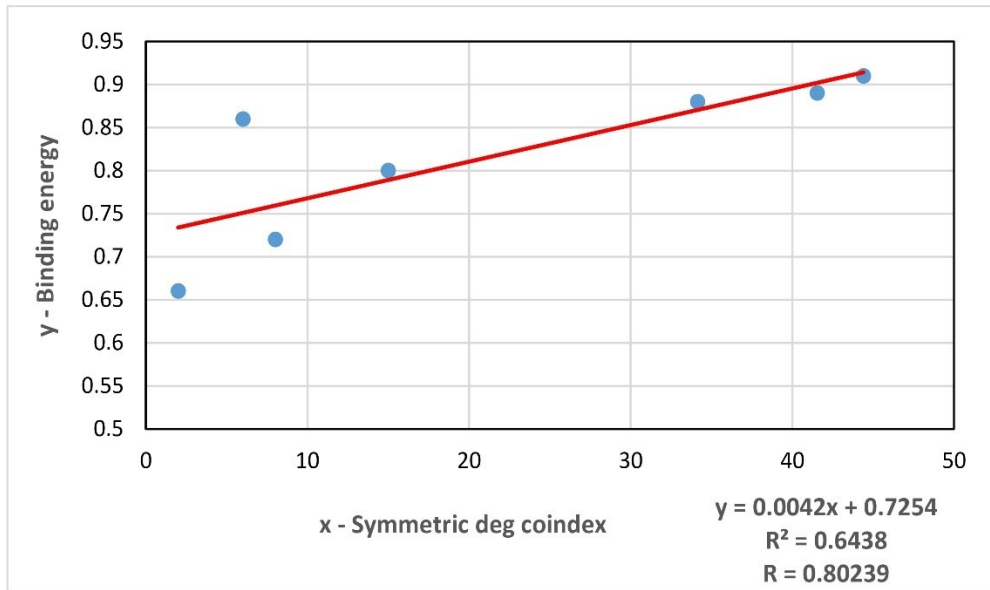


Figure 9: Scatter plot between Binding energy and \overline{SD} index of Li_n cluster

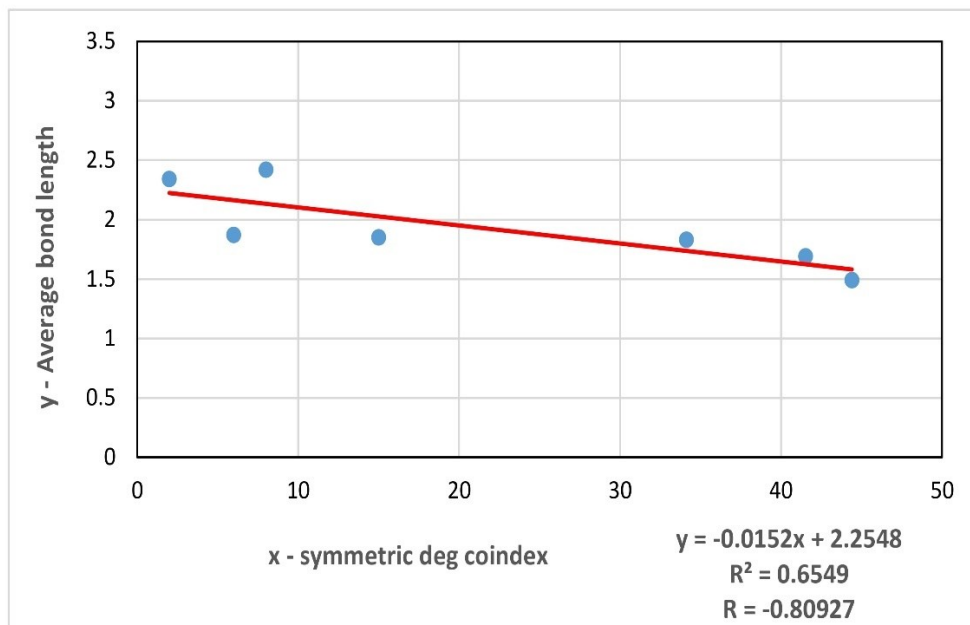


Figure 10: Scatter plot between Average bond length and \overline{SD} index of Li_n cluster

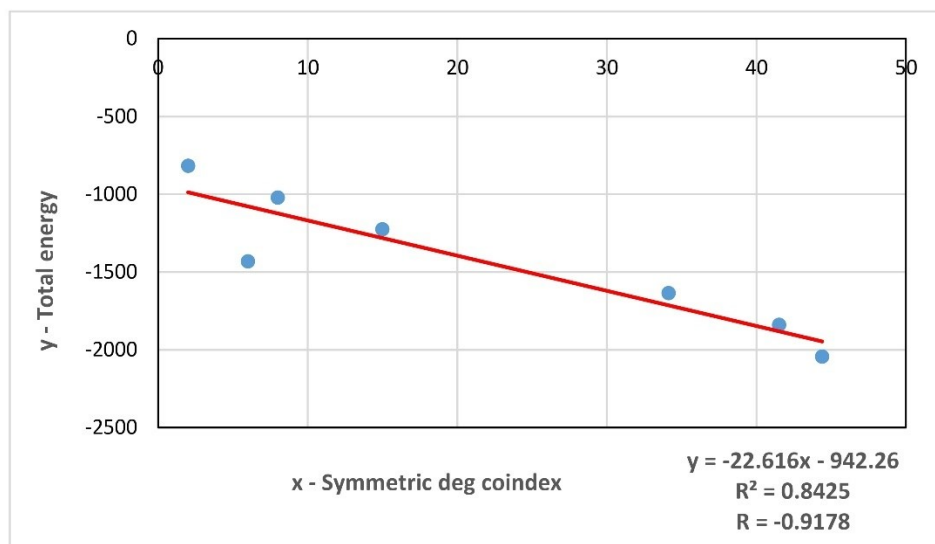


Figure 11: Scatter plot between Total energy and \overline{SD} index of Li_n cluster

Property	Correlation R	Determination R^2	SEE
Binding energy	0.8024	0.6438	0.0621
Average binding length	-0.8093	0.6549	0.2165
Total energy	-0.9178	0.8425	192.1256

Table 4: Correlation analysis of physicochemical properties of Li_n cluster with \overline{SD}

Conclusion:

In this study, we provide the symmetric deg coindex of graphs, an unique degree-based topological index. The boundaries of this index are determined after looking at the mathematical characteristics of this coindex. The Li_n cluster and certain octane isomer characteristics are examined by regression analysis.

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