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Some New Bounds on the Modified Symmetric Division Deg Index

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Abstract

The use of graph theory in the fields of chemistry, pharmacy, communication, maps, and aeronautics is significant. In order to study the properties of chemical compounds, the molecules of those compounds are modeled as graphs. Boiling point, enthalpy, π-electron energy, and molecular weight are a few examples of physical properties that are related to the geometric structure of the compound. Recently, the modified symmetric division deg (${}^{m}SDD(\mathcal{G})$, in short) index is defined as the total of all adjacent vertices in pairs $\mu\upsilon$ of the term $\sqrt{\frac{1}{2}\left(\frac{d_\mu}{d_\nu}+\frac{d_\nu}{d_\mu}\right)}$. The purpose of this article is to demonstrate the usefulness of ${}^{m}SDD(\mathcal{G})$ index through the resolution of an interdisciplinary problem describing the structure of benzenoid hydrocarbons. With the help of linear regression models, we have studied the physicochemical properties of benzenoid hydrocarbons. Strong correlations were obtained, and the bounds for the same index were subsequently established.

Keywords: topological inidces; modified symmetric division deg index; graph.

1 Introduction

The ideal tool in the hands of the chemist, graph theory involves representation, compound synthesis, and a variety of chemical operations. Additionally, because chemists are constantly interested in creating and breaking chemical bonds, various types of structures are produced. Graph theory makes it easier to extract information about a chemical compound from a mathematical model of the compound. The hydrogen atoms can be ignored when modeling a compound into a graph without losing any information about the molecule [25, 24]. Particularly in the context of chemistry applications, graph theory has proven to be a very helpful field of study.

It has a very effective tool called the topological index that offers a lot of details about a chemical compound. Degree, distance, and eccentricity are used to categorize these topological indices [2, 6]. Topological indices are measurable elements of a graph that are invariant to graph isomorphism. Topological indices are of interest because of their application in chemistry studies of the QSPR/QSAR [5, 13]. Numerous of these topological indices are based on vertices' degrees of nanocones $CNC_K[n]$ [8], nanostar dendrimers [16, 18], titania nanotubes [23], network [17, 19], silicate carbide $Si_2C_3-I[p,q]$ [3], diphenylene graph [26], succinct drug [9], aluminophosphates [28], bistar and coronal product [12], line graph of dendrimer [20], Metal organic-frameworks [21] and many more.

We begin by outlining some fundamental graph theory notation. In this article, we only take into account connected, simple, finite graphs. Let $\mathbb{V} = \mathbb{V}(\mathcal{G})$ and $\Xi = \Xi(\mathcal{G})$ vertex and edge set of the graph $\mathcal{G}$ with n vertices and m edges respectively. The degree d_μ of the vertex $\mu \in \mathbb{V}(\mathcal{G})$ is the number of edges incident to μ. Let Δ, δ are the maximum and minimum vertex degrees. The vertex (μ) is called pendent, if $d_\mu = 1$. We direct the reader to [4] for any terminologies or notations that are not clear.

The first graph invariant, named the Wiener index, to be reported as a (distance based) topological index, is defined as the halving of all vertices' distances from one another in a graph [29]. According to references [10, 14], (QSAR)/(QSAR) are generally related to the meaning of topological indices.

The Randić index [27] was introduced in 1975 and is the first and oldest degree-based topological index. It is characterized as follows:

$$R(\mathcal{G}) = \sum_{\mu\nu\in\Xi(\mathcal{G})} \frac{1}{\sqrt{d_\mu d_\nu}}. \tag{1}$$

Gutman [15] the year 1972 when he first proposed the first and second Zagreb indices, which are useful for branching questions. The variables $M_1(\mathcal{G})$ and $M_2(\mathcal{G})$, which are represented by the following:

$$M_1(\mathcal{G}) = \sum_{\mu\in\mathbb{V}(\mathcal{G})} \Big(d_\mu\Big)^2, \quad \text{and} \quad M_2(\mathcal{G}) = \sum_{\mu\nu\in\Xi(\mathcal{G})} \Big(d_\mu d_\nu\Big), \tag{2}$$

respectively. Various Zagreb index variants have been introduced in various engineering applications over the past ten years, and the modified second Zagreb index is defined by,

$$M_2^*(\mathcal{G}) = \sum_{\mu\nu\in\Xi(\mathcal{G})} \frac{1}{d_\mu d_\nu}. \tag{3}$$

In [7], the forgotten index was redefined as

$$F(\mathcal{G}) = \sum_{\mu\nu\in\Xi(\mathcal{G})} \left(d_\mu^2 + d_\nu^2\right) = \sum_{\mu\in\mathbb{V}(\mathcal{G})} \left(d_\mu\right)^3. \tag{4}$$

In [1], with the help of ratio between quadratic mean and geometric mean a new topological index is defined as $\sum_{\mu\nu\in\Xi(\mathcal{G})} \sqrt{\frac{1}{2}\left(\frac{d_\mu}{d_\nu} + \frac{d_\nu}{d_\mu}\right)}$ and named as the modified symmetric division deg index. Here we denote this index as, ${}^{m}SDD(\mathcal{G})$. That is,

$${}^{m}SDD(\mathcal{G}) = \sum_{\mu\nu\in\Xi(\mathcal{G})} \sqrt{\frac{1}{2}\left(\frac{d_\mu}{d_\nu} + \frac{d_\nu}{d_\mu}\right)} = \sum_{\mu\nu\in\Xi(\mathcal{G})} \sqrt{\frac{1}{2}\left(\frac{d_\mu^2 + d_\nu^2}{d_\mu d_\nu}\right)}.$$

In the same paper, the authors suggested that the chemical applicability of this newly defined topological index seems to be interesting. By this motivation, we studied the chemical application of ${}^{m}SDD(\mathcal{G})$ and surprisingly we found a good correlation between some properties of benzene derivatives (discussed in Section 2). Further, we found bounds for the same with known parameters (See Section 4).

2 Chemical Application of ${}^{m}SDD(\mathcal{G})$

This section focuses on framing the linear regression model for the properties listed in Table 1 boiling point (BP), enthalpy (E), and π-electron energy (π_{ele}). We use the following regression model to analyze the modified symmetric division deg index (${}^{m}SDD$) in relation to the physical characteristics:

$$\Re = {}^{m}SDD\Psi + \Upsilon, \tag{5}$$

where $\Re$ is a physical property and Ψ and Υ are the coefficient and constant, respectively. We discovered a correlation between the four physicochemical properties and the ${}^{m}SSD$ index that we proposed. In [11], the concept of maximum reverse degree energy is introduced, and a linear regression model id develop to establish the relationship between the $\pi-$ electron energy and the maximum reverse degree energy. This section presents the linear model for the index under consideration. We use the notations N for the population, S_e for standard error of the estimate, F for F-values, SF for significance F, and P-value for the probability value.

1. **The linear regression models for Boiling point**

$$BP = 20.24\ ({}^{m}SDD) - 4.46, \tag{6}$$
$$N = 22, \quad S_e = 12.5702, \quad F = 2191.2019, \quad SF = 6.4834 \times 10^{-22},$$
$$P - value = 0.0000, \quad \text{adjusted } R^2 = 0.9905.$$

2. **The linear regression models for Enthalpy**

$$E = 11.51({}^{m}SDD) + 23.31, \tag{7}$$
$$N = 22, \quad S_e = 24.0537, \quad F = 192.8371, \quad SF = 9.8906 \times 10^{-12},$$
$$P - value = 0.0000, \quad \text{adjusted } R^2 = 0.9013.$$

3. The linear regression models for π-electron energy

$$\pi_{\text{ele}} = 1.085\ (^{m}SDD) + 1.906, \tag{8}$$
$$N = 22, \quad S_e = 0.3185, \quad F = 9779.029, \quad SF = 2.21 \times 10^{-28},$$
$$P - value = 0.0000, \quad \text{adjusted } R^2 = 0.9978.$$

4. The linear regression models for Molecular wight

$$MW = 9.328\ (^{m}SDD) + 27.49, \tag{9}$$
$$N = 22, \quad S_e = 6.175, \quad F = 1920.8213, \quad SF = 2.3904 \times 10^{-21},$$
$$P - value = 0.0000, \quad \text{adjusted } R^2 = 0.9891.$$

The correlation coefficient (R) between some properties of benzene derivatives, and ^{m}SSD index is tabulated in Table 2.

Table 1: Experimental values (boiling point (BP), enthalpy (E), π-electron energy (π_{ele}) and molecular weight (MW)) of benzenoid hydrocarbons and its corresponding ^{m}SSD value.

Dervatives of benzene	BP	E	π_{ele}	MW	^{m}SSD
Benzene	80.1	75.2	8.000	78.11	6.000
Naphthalene	218	141.0	13.683	128.17	10.163
Phenanthrene	338	202.7	19.448	178.23	16.245
Anthracene	340	222.6	19.314	178.23	16.327
Chrysene	431	271.1	25.192	228.30	21.327
Benzo[a]anthracene	425	277.1	25.101	228.30	21.408
Triphenylene	429	275.1	25.275	228.30	21.245
Tetrcene	440	310.5	25.188	228.30	21.490
Benzo[a]pyrene	496	296.0	28.222	252.30	24.408
Benzo[e]pyrene	493	289.9	28.336	252.30	24.327
Perylene	497	319.2	28.245	252.30	24.237
Anthanthrene	547	323.0	31.253	276.30	27.490
Benzo[ghi]perylene	542	326.1	31.425	276.30	27.408
Dibenzi[a,c]anthracene	535	348.0	30.942	278.30	26.408
Dibenzo[a,h]anthracene	535	335.0	30.881	292.40	26.490
Dibenzo[a,j]anthracene	531	336.3	30.880	281.30	26.490
Picene	519	336.9	30.943	278.30	26.408
Coronene	590	296.7	34.572	300.40	30.490
Dienzo[a,h]pyrene	596	375.6	33.928	302.40	29.490
Dienzo[a,i]pyrene	594	366.0	33.954	302.40	29.490
Dienzo[a,l]pyrene	595	393.3	34.031	302.40	29.408
Pyrene	393	221.3	22.506	202.25	19.327

Table 2: Correlation coefficients (R) between some physicochemical properties of of benzene derivatives, and ^{m}SSD index.

Topological index	BP	E	π_{ele}	MW
^{m}SSD	0.995449329	0.952742937	0.99903747	0.994941428

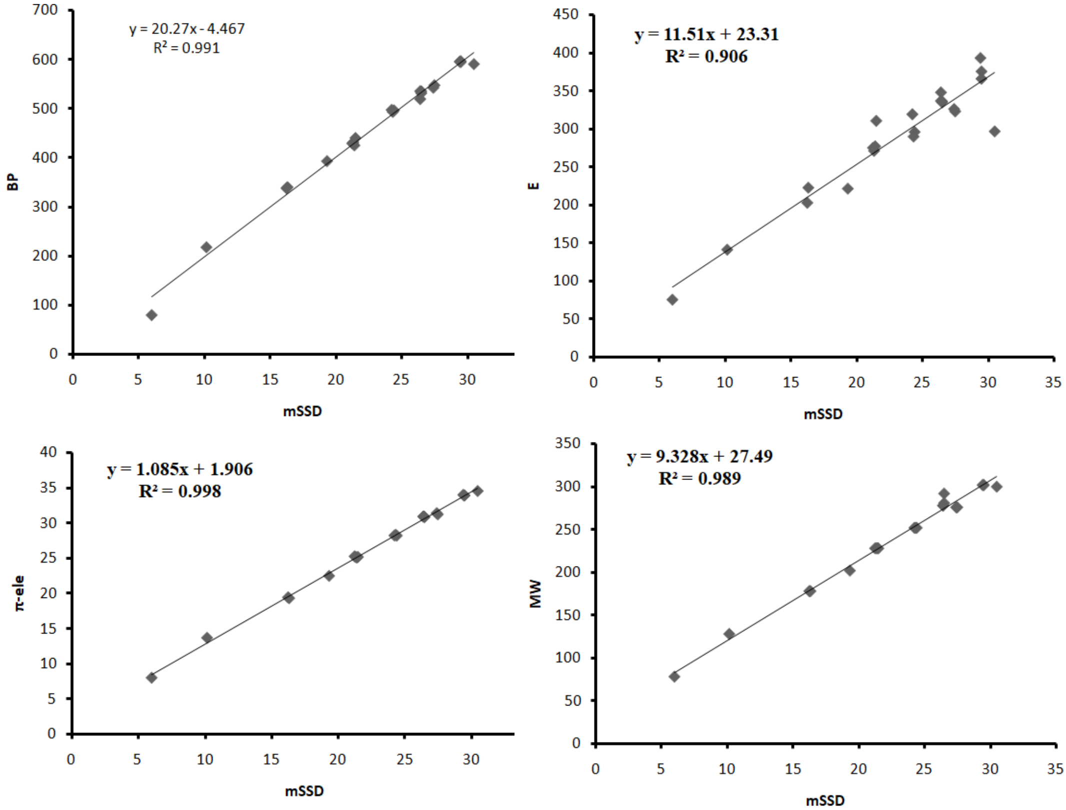

Figure 1: Correlation of ${}^{m}SDD$ index with the some properties of benzene derivatives.

3 The ${}^{m}SDD(\mathcal{G})$ Index in Various Graph

In this section we found the unique values of ${}^{m}SDD(\mathcal{G})$ for the particular graphs. The proofs are omitted as they are trivial.

Proposition 3.1. *Let $\mathcal{G}$ be a r-regular. Then,*

$$ {}^{m}SDD(\mathcal{G}) = \frac{nr}{2}. $$

Proposition 3.2. *Let C_n be a cycle graph. Then,*

$$ {}^{m}SDD(C_n) = n. $$

Proposition 3.3. *Let K_n be a complete graph. Then,*

$$ {}^{m}SDD(K_n) = \frac{n(n-1)}{2}. $$

Proposition 3.4. *Let $K_{m,n}$ be a complete bipartite graph. Then,*

$$ {}^{m}SDD(K_{m,n}) = mn\sqrt{\frac{m^2+n^2}{2mn}}. $$

Proposition 3.5. *Let P_n be a path graph. Then,*

$$ {}^{m}SDD(P_2) = 1, \quad \textit{and} \quad {}^{m}SDD(P_n) = \sqrt{5} + (n-3), \qquad n \geq 3. $$

Proposition 3.6. *Let S_n be a star graph. Then,*

$$^{m}SDD(S_n) = (n-1)\sqrt{\frac{2-2n+n^2}{2n-2}}.$$

Proposition 3.7. *Let W_n be a wheel graph. Then,*

$$^{m}SDD(W_n) = (n-1) + (n-1)\sqrt{\frac{n^2-2n+10}{6(n-1)}}, \qquad (n \geq 4).$$

4 Bounds

Here, we establish bounds for ^{m}SDD index.

Lemma 4.1. [22] *Let $F(x,y) = \dfrac{x}{y} + \dfrac{y}{x}$, and real number a and b satisfied that $0 < a \leq x \leq y \leq b$. Then $2 \leq F(x,y) \leq \dfrac{a}{b} + \dfrac{b}{a}$ with left equality holds if and only if $x = y$ and right equality holds if and only if $x = a,\ y = b$.*

Theorem 4.1. *Let $\mathcal{G}$ be a simple connected graph of order $n(\geq 3)$ and size m. Then,*

$$m \leq {}^{m}SDD(\mathcal{G}) \leq \left(\frac{\Delta}{\delta}\right) m.$$

The equality is true iff $\mathcal{G}$ is a regular graph.

Proof. For every edge $e = \mu\nu \in \Xi(\mathcal{G})$, we have $\delta \leq d_\mu \leq \Delta \implies 2\delta^2 \leq d_\mu^2 + d_\nu^2 \leq 2\Delta^2$ and so,

$$\begin{aligned} ^{m}SDD(\mathcal{G}) &= \sum_{\mu\nu \in \Xi(\mathcal{G})} \sqrt{\frac{1}{2}\left(\frac{d_\mu^2 + d_\nu^2}{d_\mu d_\nu}\right)} \\ &\leq \Delta \sum_{\mu\nu \in \Xi(\mathcal{G})} \frac{1}{\sqrt{d_\mu d_\nu}} \\ &= \left(\frac{\Delta}{\delta}\right) m. \end{aligned}$$

By Lemma 4.1 (left equality), we have the following,

$$\begin{aligned} &\frac{d_\mu^2 + d_\nu^2}{d_\mu d_\nu} \geq 2 \\ \implies &\sqrt{\frac{1}{2}\left(\frac{d_\mu^2 + d_\nu^2}{d_\mu d_\nu}\right)} \geq 1, \end{aligned}$$

and by taking summation over the all edges we arrive at,

$$^{m}SDD(\mathcal{G}) \geq m.$$

Thus the required result. It is obvious that inequality is true iff $\mathcal{G}$ is a regular graph. □

Theorem 4.2. *Let $\mathcal{G}$ be a simple connected with m edges. Then,*

$$^{m}SDD(\mathcal{G}) \leq \sqrt{\frac{mF(\mathcal{G})}{2\delta^2}}.$$

Proof. We have $\delta \leq d_\mu \leq \Delta$,

$$\begin{aligned}(\,^{m}SDD(\mathcal{G})\,)^2 &= \left(\sum_{\mu\nu\in\Xi(\mathcal{G})}\sqrt{\frac{d_\mu^2+d_\nu^2}{2d_\mu d_\nu}}\right)^2\\ &= \frac{1}{2}\left(\sum_{\mu\nu\in\Xi(\mathcal{G})}\sqrt{\frac{d_\mu^2+d_\nu^2}{d_\mu d_\nu}}\right)^2.\end{aligned}$$

By Cauchy-Schwarz inequality, we have

$$\begin{aligned}(\,^{m}SDD(\mathcal{G})\,)^2 &\leq \frac{1}{2}\sum_{\mu\nu\in\Xi(\mathcal{G})}[d_\mu^2+d_\nu^2]\sum_{\mu\nu\in\Xi(\mathcal{G})}\frac{1}{d_\mu d_\nu}\\ &= \frac{m}{2}\frac{F(\mathcal{G})}{\delta^2}.\end{aligned}$$

□

Theorem 4.3. *Let $\mathcal{G}$ be a simple connected graph with m size. Then,*

$$\sqrt{\delta^2\left(M_2^*(\mathcal{G})+\frac{m(m-1)}{\Delta^2}\right)} \leq \,^{m}SDD(\mathcal{G}) \leq \sqrt{\Delta^2\left(M_2^*(\mathcal{G})+\frac{m(m-1)}{\delta^2}\right)}.$$

Proof. From the definition we have,

$$\begin{aligned}(\,^{m}SDD(\mathcal{G})\,)^2 &= \sum_{u_iv_j\in\Xi(\mathcal{G})}\left(\sqrt{\frac{d_{u_i}^2+d_{v_j}^2}{2d_{u_i}d_{v_j}}}\right)^2 + 2\sum_{u_iv_j\neq u_pv_q\in\Xi(\mathcal{G})}\left(\sqrt{\frac{d_{u_i}^2+d_{v_j}^2}{2d_{u_i}d_{v_j}}}\sqrt{\frac{d_{u_p}^2+d_{v_q}^2}{2d_{u_p}d_{v_q}}}\right)\\ &\leq \sum_{u_iv_j\in\Xi(\mathcal{G})}\frac{\Delta^2}{d_{u_i}d_{v_j}} + 2\sum_{u_iv_j\in\Xi(\mathcal{G})}\left(\frac{\Delta}{\delta}\right)\left(\frac{\Delta}{\delta}\right)\\ &\leq \Delta^2\sum_{u_iv_j\in\Xi(\mathcal{G})}\frac{1}{d_{u_i}d_{v_j}} + \left(2\frac{\Delta^2}{\delta^2}\right)\left(\frac{m(m-1)}{2}\right)\\ &\leq \Delta^2\left(M_2^*(\mathcal{G})+\frac{m(m-1)}{\delta^2}\right).\end{aligned}$$

Similarly,

$$(\,^{m}SDD(\mathcal{G})\,)^2 \geq \delta^2\left(M_2^*(\mathcal{G})+\frac{m(m-1)}{\Delta^2}\right).$$

□

Theorem 4.4. *Let $\mathcal{G}$ be a simple connected graph of order $n(\geq 3)$ and size m. Then,*

$$\frac{\delta}{\Delta} < \,^{m}SDD(\mathcal{G}) < \sqrt{2}m\Delta.$$

Proof.

$$\begin{aligned}
{}^{m}SDD(\mathcal{G}) &= \sum_{\mu\nu\in\Xi(\mathcal{G})} \sqrt{\frac{d_\mu^2+d_\nu^2}{2d_\mu d_\nu}}\\
&> \frac{\sum\limits_{\mu\nu\in\Xi(\mathcal{G})} \sqrt{d_\mu^2+d_\nu^2}}{\sum\limits_{\mu\nu\in\Xi(\mathcal{G})} \sqrt{2d_\mu d_\nu}},
\end{aligned}$$

provided $2\delta^2 \leq d_\mu^2+d_\nu^2 \leq 2\Delta^2, \forall\, u,v \in \Xi(\mathcal{G})$. We get,

$$\frac{\sum\limits_{\mu\nu\in\Xi(\mathcal{G})} \sqrt{d_\mu^2+d_\nu^2}}{\sum\limits_{\mu\nu\in\Xi(\mathcal{G})} \sqrt{2d_\mu d_\nu}} > \frac{\delta}{\Delta}.$$

Since,

$$\begin{aligned}
{}^{m}SDD(\mathcal{G}) &= \sum_{\mu\nu\in\Xi(\mathcal{G})} \sqrt{\frac{d_\mu^2+d_\nu^2}{d_\mu d_\nu}}\\
&< \sum_{\mu\nu\in\Xi(\mathcal{G})} \sqrt{d_\mu^2+d_\nu^2}\\
&= \sqrt{\sum_{\mu\nu\in\Xi(\mathcal{G})}(1) \sum_{\mu\nu\in\Xi(\mathcal{G})} [d_\mu^2+d_\nu^2]}\\
&= \sqrt{2m^2\Delta^2} = \sqrt{2}m\Delta.
\end{aligned}$$

□

Theorem 4.5. *Let $\mathcal{G}$ be a simple connected graph having m edges, p pendent vertices. Then,*

$$\frac{\delta}{\Delta}(m-p) + \sqrt{\frac{1+\delta^2}{2\Delta}}p \leq {}^{m}SDD(\mathcal{G}) \leq \frac{\delta}{\Delta}(m-p) + \sqrt{\frac{1+\delta^2}{2\Delta}}p.$$

Proof.

$$\begin{aligned}
{}^{m}SDD(\mathcal{G}) &= \sum_{\mu\nu\in\Xi(\mathcal{G}),\ d_\mu,d_\nu\neq 1} \left(\sqrt{\frac{d_\mu^2+d_\nu^2}{2d_\mu d_\nu}}\right) + \sum_{\mu\nu\in\Xi(\mathcal{G}),d_\mu=1} \left(\sqrt{\frac{d_\mu^2+d_\nu^2}{2d_\mu d_\nu}}\right)\\
&\leq \sqrt{\frac{1}{2}\left(\frac{2\Delta^2}{\delta^2}\right)}(m-p) + \sqrt{\frac{1}{2}\left(\frac{1+\Delta^2}{\delta}\right)}p\\
&= \frac{\Delta}{\delta}(m-p) + \sqrt{\frac{1+\Delta^2}{2\delta}}p.
\end{aligned}$$

Similarly,

$${}^{m}SDD(\mathcal{G}) \geq \frac{\delta}{\Delta}(m-p) + \sqrt{\frac{1+\delta^2}{2\Delta}}p.$$

□

Lemma 4.2. [7] (*Polya-Szego inequality*) *Assume that* $x_i, y_i \in \mathbb{R}^+$, *for* $i = 1, 2, \dots, m$ *with* $p \le x_i \le P$ *and* $q \le y_i \le Q$, *then,*

$$\sum_{i=1}^{m} y_i^2 \sum_{i=1}^{m} x_i^2 \le \frac{1}{4}\left(\sqrt{\frac{PQ}{pq}} + \sqrt{\frac{pq}{PQ}}\right)^2 \left(\sum_{i=1}^{m} x_i y_i\right)^2.$$

Theorem 4.6. *Let* $\mathcal{G}$ *be a simple connected graph with order* n *and size* m. *Then,*

$$^{m}SDD(\mathcal{G}) \ge \frac{m\left(\frac{\delta}{\Delta}\right)}{\frac{1}{2}\left(\frac{\Delta}{\delta} + \frac{\delta}{\Delta}\right)}.$$

Proof. Choosing $y_i = \sqrt{\dfrac{d_\mu^2 + d_\nu^2}{2d_\mu d_\nu}}$, $x_i = 1$, $P = \sqrt{\dfrac{\Delta}{\delta}}$, $q = \sqrt{\dfrac{\delta}{\Delta}}$, and $Q = q = 1$ in Lemma 4.2. Then we get,

$$\sum_{\mu\nu \in \Xi(\mathcal{G})} \frac{d_\mu^2 + d_\nu^2}{2d_\mu d_\nu} \sum_{\mu\nu \in \Xi(\mathcal{G})} (1) \le \frac{1}{4}\left(\sqrt{\frac{\frac{\Delta}{\delta}}{\frac{\delta}{\Delta}}} + \sqrt{\frac{\frac{\delta}{\Delta}}{\frac{\Delta}{\delta}}}\right)^2 \left(\sum_{\mu\nu \in \Xi(\mathcal{G})} \sqrt{\frac{d_\mu^2 + d_\nu^2}{2d_\mu d_\nu}}\right)^2$$

$$m\left(\sum_{\mu\nu \in \Xi(\mathcal{G})} \frac{\delta^2}{\Delta^2}\right) \le \frac{1}{4}\left(\frac{\Delta}{\delta} + \frac{\delta}{\Delta}\right)^2 \left(^{m}SDD(\mathcal{G})\right)^2$$

$$\left(m\frac{\delta}{\Delta}\right)^2 \le \left[\frac{1}{2}\left(\frac{\Delta}{\delta} + \frac{\delta}{\Delta}\right)\right]^2 \left(^{m}SDD(\mathcal{G})\right)^2.$$

The required result can be achieved by simplifying. □

Lemma 4.3 (Ozeki inequality). [7] *If* x_i *and* y_i *are positive* n*-tuples, then* P, p, Q, *and* q *are positive numbers such that,* $0 < p \le x_i \le P$, $0 < q \le y_i \le Q$, *and* $1 \le i \le n$. *Then,*

$$\sum_{i=1}^{n} x_i^2 \sum_{i=1}^{n} y_i^2 - \left(\sum_{i=1}^{n} x_i y_i\right)^2 \le \frac{1}{4} n^2 (PQ - pq).$$

Theorem 4.7. *Let* $\mathcal{G}$ *be a simple connected graph with order* n *and size* m. *Then,*

$$\sqrt{\delta^2 m M_2^*(\mathcal{G}) - \frac{n^2}{4}\left(\frac{\Delta}{\delta} - \frac{\delta}{\Delta}\right)} \le {}^{m}SDD(\mathcal{G}).$$

Proof. Choosing $x_i = \sqrt{d_\mu^2 + d_\nu^2}$, $y_i = \dfrac{1}{\sqrt{2d_\mu d_\nu}}$, $P = \sqrt{2}\Delta$, $p = \sqrt{2}\delta$, $Q = \dfrac{1}{\sqrt{2}\delta}$, and $q = \dfrac{1}{\sqrt{2}\Delta}$ in lemma 4.3. We get,

$$\sum_{\mu\nu\in\Xi(\mathcal{G})}\left(d_\mu^2+d_\nu^2\right)\sum_{i=1}^{n}\frac{1}{2d_\mu d_\nu}-\left(\sum_{\mu\nu\in\Xi(\mathcal{G})}\sqrt{\frac{d_\mu^2+d_\nu^2}{2d_\mu d_\nu}}\right)^2\leq\frac{n^2}{4}\left(\frac{\Delta}{\delta}-\frac{\delta}{\Delta}\right)$$

$$\delta^2\left(\sum_{\mu\nu\in\Xi(\mathcal{G})}(1)\right)M_2^*(\mathcal{G})-\left({}^{m}SDD(\mathcal{G})\right)^2\leq\frac{n^2}{4}\left(\frac{\Delta}{\delta}-\frac{\delta}{\Delta}\right)$$

$$\delta^2 m M_2^*(\mathcal{G})-\left({}^{m}SDD(\mathcal{G})\right)^2\leq\frac{n^2}{4}\left(\frac{\Delta}{\delta}-\frac{\delta}{\Delta}\right).$$

On rearranging we get the required result. □

5 Conclusion

To analyze many physical and chemical properties of compounds without using costly and time-consuming laboratory experiments, QSPR analysis, which is based on topological descriptors, is a very useful statistical method. It is interesting to note that when ${}^{m}SDD$ values are correlated with experimental values of benzenoid hydrocarbons, such as boiling point (BP), enthalpy (E), molecular weight (MW), and π-electron energy (π_{ele}), ${}^{m}SSD$ has demonstrated a strong correlation with correlation coefficient (see Table 2 and Figure 1), and there are linear regression models that can be seen in equations (6), (7), (8), and (9).

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Conflicts of Interest The authors declare no conflict of interest.

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