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Minimum Vertex Degree Index for Graphs

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ABSTRACT: In this research work, we introduce the notion of new topological index called Minimum Vertex Degree Index ($MVDI$), for a graph G and obtain $MVDI$ for few graphs. Also, we obtain $MVDI$ for few chemical structures and develop a report comprising data analysis for properties of lower alkanes.

Key Words: Minimum vertex degree index, elliptic delta and modified elliptic delta.

Contents

1. Introduction

This entire manuscript studies graphs, that are connected, simple, undirected and finite, which are given in [7] by F.Harary. Here vertex set is represented by $V(G)$ and edge set by $E(G)$ for a graph G with n vertices. We represent degree of vertex v_i as $d(v_i)$. The graph energy and the topological index for graphs are very attractive due their importance in mathematical chemistry. In the research field of drug development, the task of topological indices is well defined. In the process of drug invention technology, a sequence of definitions for topological indices are discussed. There exists many distance based and degree based topological indices defined for graphs.

A graphical structure attains numerical value through a topological index. A huge variety of graph indices are introduced and their applications in various disciplines are studied in [1,2,3,4,5,6,8,9,10,11,12, 13,14,15,16,17,20,21]. These indices are graph invariant and are used for QSPR (Quantitative Structure Property Relationship) and QSAR (Quantitative Structure Activity Relationship).

We consider the following definitions from papers of V. R. Kulli [18,19], in the process of developing the paper.

The δ vertex degree at vertex u is defined as

$$\delta_u = d_u - \delta(G) + 1$$

Here $\delta(G)$ represents minimum degree among the vertices of G.

Definition 1.1 The elliptic delta index of the graph G is defined as,

$$E\delta(G) = \sum_{uv \in E(G)} (\delta_u + \delta_v)\sqrt{\delta_u^2 + \delta_v^2}$$

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Definition 1.2 The modified elliptic delta index of the graph G is defined as,

$$^{m}E\delta(G) = \sum_{uv \in E(G)} \frac{1}{(\delta_u + \delta_v)\sqrt{\delta_u^2 + \delta_v^2}}$$

Motivated by the above works, we introduce a new topological index called Minimum Vertex Degree Index ($MVDI$), in section 2 and compute ($MVDI$) for few special and standard graphs. In section 3 we compute $MVDI$ for chemical structure of certain networks. In section 4 we give QSPR analysis for physical properties of lower alkanes and also give regression models for the analysis.

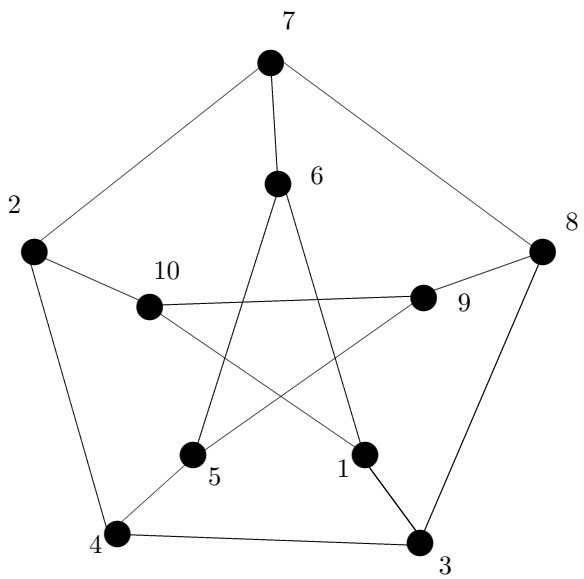
2. Definition and Computation of Minimum Vertex Degree Index of Some Special and Standard Graphs

Let G be a simple graph with $\{v_1, v_2, ..., v_n\}$ as vertex set and $d(u_i)$ and $d(v_i)$ denote the degree of u_i and v_i respectively for, $i = 1, 2, 3, ..., n$. Then, we define $MVDI$ as follows,

$$MVDI(G) = \sum_{u_i v_i \in E} min[d(u_i), d(v_i)] \tag{2.1}$$

Using the above definition, we have the following computations:

Example 1:



The $MVDI$ for above Peterson graph is 30.

Now we give MVDI for few standard graphs, 1. For a path P_n with n vertices we have,

$$MVDI(P_n) = 2n - 4.$$

2. For a cycle C_n with n vertices we have,

$$MVDI(C_n) = 2|E| = 2n.$$

3. For a complete graph K_n with n vertices we have,

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

4. For a fan graph F_n with n vertices we have,

$$MVDI(F_n) = 6(n-1) - 1.$$

5. For a Star graph S_n with n vertices we have,

$$MVDI(S_n) = (n-1)^2.$$

6. For a Double Star graph $S_n \times S_n$ with n vertices we have,

$$MVDI(S_n \times S_n) = (n-2) + 4.$$

3. Computation of Minimum Vertex Degree Index for Chemical Structure of Certain Networks

3.1. Minimum Vertex Degree Index for Silicate Network:

Among the minerals found in nature silicates are accepted as complicated, largest and interesting compound. They are tetrahedron denoted by SiO_4. When we represent it in two-dimensional plane, we see it as a ring formed by tetrahedrons, which are joined by oxygen nodes and we notice it as a sheetlike structure.

When we represent silicate network (SL_n) as a graph G, the number of silicon nodes equals the product of number of nodes of SL_n, also the number of edges in G is $6 \times 6n^2$=$36n^2$. Based on the degree at the vertex, it has the following three types of edges,

$$E_{3,3} = \{u_i v_i \in E(G) \mid d(u_i) = d(v_i) = 3\}, \mid E_{3,3} \mid = 6n.$$

$$E_{3,6} = \{u_i v_i \in E(G) \mid d(u_i) = 3, d(v_i) = 6\}, \mid E_{3,6} \mid = 18n^2 + 6n.$$

$$E_{6,6} = \{u_i v_i \in E(G) \mid d(u_i) = 6, d(v_i) = 6\}, \mid E_{6,6} \mid = 18n^2 - 12n.$$

Theorem 3.1 *Let G be the graphical representation of a Silicate Network SL_n. Then,*

$$MVDI(G) = 162n^2 - 36n.$$

Proof: *By definition we have,*

$$MVDI(G) = \sum_{uv \in E} min[d(u_i), d(v_i)] \tag{3.1}$$

$$= 162n^2 - 36n.$$

□

Also we have the following bounds for G which represents SL_n,

(i) $MVDI(G) < E\delta(G)$

i.e, $162n^2 - 36n < (90\sqrt{17} + 576\sqrt{2})n^2 + (30\sqrt{17} - 372\sqrt{2})n$.

(ii) $MVDI(G) >^m E\delta(G)$

i.e, $162n^2 - 36n > \frac{6n}{2\sqrt{2}} + \frac{18n^2+6n}{5\sqrt{17}} + \frac{18n^2-12n}{32\sqrt{2}}$.

3.2. Minimum Vertex Degree Index for Honeycomb Network

A honeycomb network is a regular network (HC_n) with a hexagonal topology that can be constructed in any dimension. Honeycomb networks are often used to study complex systems and their properties. The applications of Honeycomb networks include Material science, Physics, Computer science, and Communication network design. In [19] V.R. Kulli obtained that the graphical structure of HC_n has $6n^2$ vertices and $9n^2 - 3n$ edges. Based on the degree at the vertex, it has the following three types of edges,

$$E_{2,2} = \{u_iv_i \in E(G) \mid d(u_i) = d(v_i) = 2\}, \mid E_{2,2} \mid = 6.$$

$$E_{2,3} = \{u_iv_i \in E(G) \mid d(u_i) = 2, d(v_i) = 3\}, \mid E_{2,3} \mid = 12n - 12.$$

$$E_{3,3} = \{u_iv_i \in E(G) \mid d(u_i) = d(v_i) = 3\}, \mid E_{3,3} \mid = 9n^2 - 15n + 6.$$

Theorem 3.2 *Let G be the graphical representation of a honeycomb network HC_n. Then,*

$$MVDI(G) = 27n^2 - 21n + 6.$$

Proof: *By definition we have,*

$$MVDI(G) = \sum_{u_iv_i \in E} min[d(u_i), d(v_i)] \tag{3.2}$$

$$= 27n^2 - 21n + 6.$$

□

Also we have the following bounds for G which represents HC_n,

(i) $MVDI(G) < E\delta(G)$

i.e, $27n^2 - 21n + 6 < 72\sqrt{2}n^2 + (36\sqrt{5} - 120\sqrt{2})n + 60\sqrt{2} - 36\sqrt{5}$.

(ii) $MVDI(G) >^m E\delta(G)$

i.e, $27n^2 - 21n + 6 > \frac{6}{2\sqrt{2}} + \frac{12n-12}{3\sqrt{5}} + \frac{9n^2-15n+6}{8\sqrt{2}}$.

3.3. Minimum Vertex Degree Index for Oxide Network:

An oxide network (OX_n) is a network that is created by removing all the silicon nodes in a silicate network, hence the diameter of both SL_n and OX_n are same. An n-dimensional oxide network is represented by OX_n. Oxide networks are important for studying the metric and structural properties of silicate networks.

Let G be the graph of an oxide network OX_n. The graph G has $9n^2 + 3n$ vertices and $18n^2$ edges. Based on the degree at the vertex, it has the following two types of edges,

$$E_{2,4} = \{u_iv_i \in E(G) \mid d_G(u_i) = 2, d_G(v_i) = 4\}, \mid E_{2,4} \mid = 12n.$$

$$E_{4,4} = \{u_iv_i \in E(G) \mid d_G(u_i) = d_G(v_i) = 4\}, \mid E_{4,4} \mid = 18n^2 - 12n.$$

Theorem 3.3 *Let G be the graphical representation of an oxide network OX_n. Then,*

$$MVDI(G) = 72n^2 - 24n.$$

Proof: *By definition we have,*

$$MVDI(G) = \sum_{u_iv_i \in E} min[d(u_i), d(v_i)] \tag{3.3}$$

$$= 72n^2 - 24n.$$

□

Also we have the following bounds for G which represents OX_n,

(i) $MVDI(G) < E\delta(G)$

i.e, $72n^2 - 24n < 162\sqrt{2}n^2 + (24\sqrt{10} - 54\sqrt{2})n$.

(ii) $MVDI(G) >^m E\delta(G)$

i.e, $72n^2 - 24n > \frac{6n}{4\sqrt{10}} + \frac{9n^2-3n}{18\sqrt{2}}$.

3.4. Minimum Vertex Degree Index for Hexagonal Network:

In graph theory, a hexagonal network is a network that is modeled by a planar graph and is based on a triangular plane tessellation. This means that the network is made up of equilateral triangles, with each node having up to six neighbours. In a hexagonal network the total count of number of edges and vertices are $(3n(n-1)+1)$ and $(9n-15)n+6)$ respectively. Based on the degree at the vertex, it has the following five types of edges,

$$E_{3,4} = \{u_iv_i \in E(G) \mid d(u_i) = 3, d_G(v_i) = 4\}, \mid E_{3,4} \mid = 12.$$

$$E_{3,6} = \{u_iv_i \in E(G) \mid d(u_i) = 3, d(v_i) = 6\}, \mid E_{3,6} \mid = 6.$$

$$E_{4,4} = \{u_iv_i \in E(G) \mid d(u_i) = d(v_i) = 4\}, \mid E_{4,4} \mid = 16n - 18.$$

$$E_{4,6} = \{u_iv_i \in E(G) \mid d(u_i) = 4, d(v_i) = 6\}, \mid E_{4,6} \mid = 12n - 24.$$

$$E_{6,6} = \{u_iv_i \in E(G) \mid d(u_i) = d(v_i) = 6\}, \mid E_{6,6} \mid = 9n^2 - 33n + 30.$$

Theorem 3.4 *Let G be the graphical representation of a Hexagonal Network HX_n. Then,*

$$MVDI(G) = 54n^2 - 126n + 66.$$

Proof: *By definition we have,*

$$MVDI(G) = \sum_{u_iv_i \in E} min[d(u_i), d(v_i)] \tag{3.4}$$

$$= 54n^2 - 126n + 66.$$

□

Also we have the following bounds for G which represents HX_n,

(i) $MVDI(G) < E\delta(G)$

i.e, $54n^2 - 126n + 66 < 288\sqrt{2}n^2 + (144\sqrt{5} - 1008\sqrt{2})n + 30\sqrt{17} - 252\sqrt{5} + 816\sqrt{2}$.

(ii) $MVDI(G) >^m E\delta(G)$

i.e, $54n^2 - 126n + 66 > \frac{12}{3\sqrt{5}} + \frac{6}{5\sqrt{17}} + \frac{6n-18}{8\sqrt{2}} + \frac{12n-24}{12\sqrt{5}} + \frac{9n^2-33n+30}{32\sqrt{2}}$.

4. A QSPR Analysis for MVDI

In this section, we carry out QSPR analysis of molecular structures of graphs using MVDI for properties of lower alkanes. The MVDI for molecular structures of graphs of lower alkanes are obtained further they are tabulated in the Table 1. For the analysis, we used Practical values of the properties - surface tensions (st) dyne cm^{-1}, critical temperatures $(ct)C$, molar refractions (mr) cm^3, critical pressures (cp) atm, heats of vaporization (hv) kJ molar volumes (mv) cm^3, and boiling points $(bp)C$ for lower alkanes, presented in [17].

Following Table 1 shows the corelation between the properties of lower alkanes and MVDI. The corelation coefficient r is a measure of how strongly a pair of variables are related. It usually varies among -1 and +1. If r is nearer to +1 then we say that variables are set to be strongly, positively and linearly proportional. If r is nearer to -1 then we say that variables are set to be strongly, negatively and linearly inversely proportional. If r close to zero or r is equal to zero, then we conclude that there is no relationship between the variables. (we observe from Table 1 that properties of lower alkanes are positively proportional and is closer to the value+1)

Table 1: Minimum Vertex Degree Index of low alkanes

Alkane	$MVDI$	*Alkane*	$MVDI$
2,3,4-Trimethylpentane	*11*	*Ethane*	*1*
Nonane	*14*	*Propane*	*4*
2-Methyloctane	*13*	*Butane*	*4*
3-Methyloctane	*13*	*2-Methylpropane*	*3*
4-Methyloctane	*13*	*Pentane*	*6*
3-Ethylheptane	*13*	*2-Methylbutane*	*5*
4-Ethylheptane	*13*	*2,2-Dimethylpropane*	*4*
2,2-Dimethylheptane	*12*	*Hexane*	*8*
2,3-Dimethylheptane	*13*	*2-Methylpentane*	*7*
2,3,4-Trimethylpentane	*11*	*Ethane*	*1*
Nonane	*14*	*Propane*	*4*
2-Methyloctane	*13*	*Butane*	*4*
3-Methyloctane	*13*	*2-Methylpropane*	*3*
4-Methyloctane	*13*	*Pentane*	*6*
3-Ethylheptane	*13*	*2-Methylbutane*	*5*
4-Ethylheptane	*13*	*2,2-Dimethylpropane*	*4*
2,2-Dimethylheptane	*12*	*Hexane*	*8*
2,3-Dimethylheptane	*13*	*2-Methylpentane*	*7*
2,4-Dimethylheptane	*12*	*3-Methylpentane*	*7*

Alkane	$MVDI$	*Alkane*	$MVDI$
2,5-Dimethylheptane	*12*	*2,2-Dimethylbutane*	*6*
2,6-Dimethylheptane	*12*	*2,3-Dimethylbutane*	*7*
3,3-Dimethylheptane	*12*	*Heptane*	*9*
3,4-Dimethylheptane	*13*	*2-Methylhexane*	*9*
3,5-Dimethylheptane	*12*	*3-Methylhexane*	*9*
4,4-Dimethylheptane	*13*	*3-Ethylhexane*	*11*
3-Ethyl-2-methylhexane	*13*	*2,2-Dimethylpentane*	*8*
4-Ethyl-2-methylhexane	*12*	*2,3-Dimethylpentane*	*9*
3-Ethyl-3-methylhexane	*12*	*2,4-Dimethylpentane*	*8*
3-Ethyl-4-methylhexane	*13*	*3,3-Dimethylpentane*	*8*
2,2,3-Trimethylhexane	*12*	*2,3,3-Trimethylbutane*	*8*
2,2,4-Trimethylhexane	*11*	*Octane*	*12*
2,2,5-Trimethylhexane	*11*	*2-Methylheptane*	*11*
2,3,3-Trimethylhexane	*12*	*3-Methylheptane*	*11*
2,3,4-Trimethylhexane	*13*	*4-Methylheptane*	*11*
2,3,5-Trimethylpentane	*11*	*4-Ethylhexane*	*11*
2,4,4-Trimethylhexane	*11*	*2,2-Dimethylhexane*	*10*
3,3,4-Trimethylhexane	*12*	*2,3-Dimethylhexane*	*11*
3,3,4-Trimethylhexane	*12*	*2,4-Dimethylhexane*	*10*
3,3-Diethylpentane	*12*	*2,5-Dimethylhexane*	*10*
2,2-Dimethyl-3-ethylpentane	*12*	*3,3-Dimethylhexane*	*10*
2,3-Dimethyl-3-ethylpentane	*12*	*3-Ethyl-2-methylpentane*	*11*
2,4-Dimethyl-3-ethylpentane	*13*	*3,4-Dimethylhexane*	*11*
2,2,3,3-Tetramethylpentane	*12*	*3-Ethyl-3-methylpentane*	*10*
2,2,3,4-Tetramethylpentane	*12*	*2,2,3-Trimethylpentane*	*10*
2,2,4,4-Tetramethylpentane	*10*	*2,2,4-Trimethylpentane*	*9*
2,3,3,4-Tetramethylpentane	*12*	*2,3,3-Trimethylpentane*	*10*

Table 2: r, r^2 and p-value between MVDI and physical properties

Y	r	r^2	*value*	*Std error*
Bp	0.9525	0.9073	$2.5361e-36$	0.5355
Mv	0.8908	0.7935	$1.2124e-24$	0.4413
Mr	0.9131	0.8337	$8.3913e-28$	0.1205
Hv	0.9572	0.9163	$8.2717e-38$	0.0872
Ct	0.9271	0.8595	$2.9028e-30$	0.8012
Cp	-0.8167	0.6671	$1.1765e-17$	0.0850
St	0.9023	0.8141	$8.3752e-26$	0.0504

Regression models The linear model for the properties of the lower alkanes with $MVDI$ is provided by the following equations.

$$y_{Bp} = 13.7131MVDI - 30.8657 \tag{4.1}$$
$$y_{Mv} = 7.0810MVDI + 87.5205 \tag{4.2}$$
$$y_{Mr} = 2.2085MVDI + 16.0566 \tag{4.3}$$
$$y_{Hv} = 2.3626MVDI + 13.7306 \tag{4.4}$$
$$y_{Ct} = 16.2226MVDI + 119.1618 \tag{4.5}$$
$$y_{Cp} = -0.9847MVDI + 36.7448 \tag{4.6}$$
$$y_{St} = 0.8571MVDI + 11.7596 \tag{4.7}$$

The variables are shown to coincide with one another in the following graphs. The coefficient of determination is high if the model's traces are closer to the real values. Therefore, there is no need to improve the current state of the model.

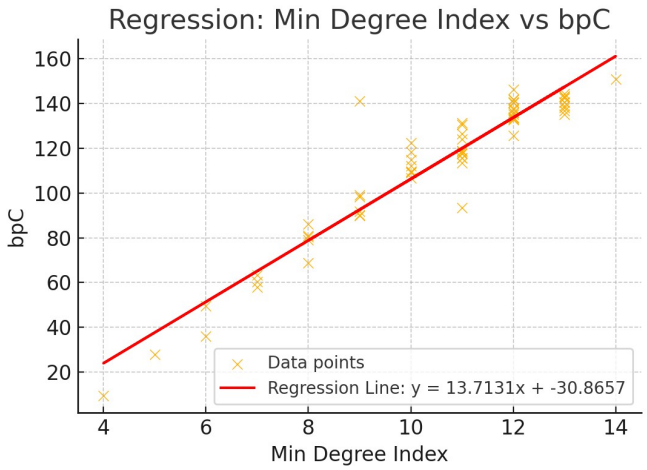


Figure 1: Regression model for *bp*

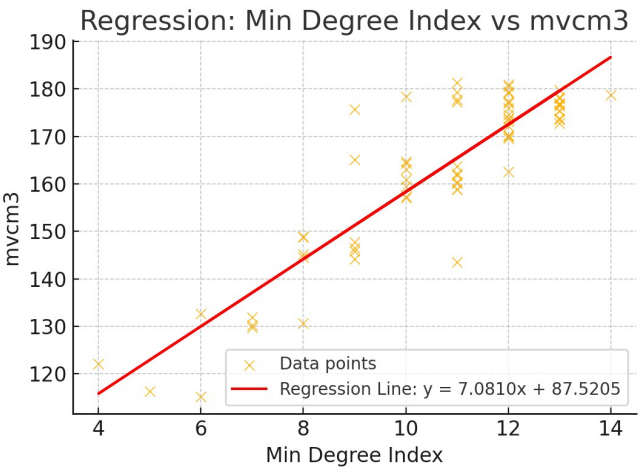


Figure 2: Regression model for *mv*

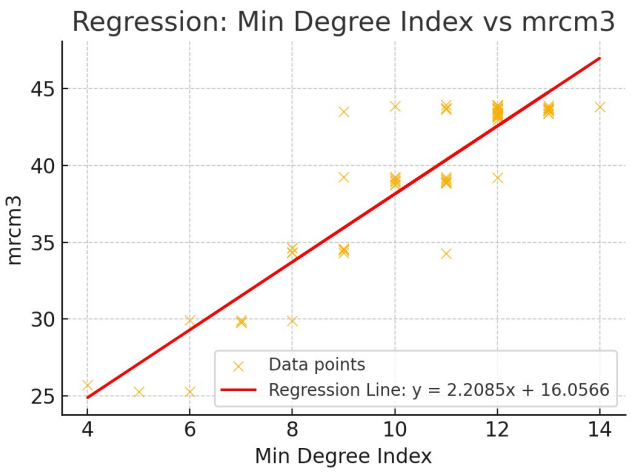


Figure 3: Regression model for *mr*

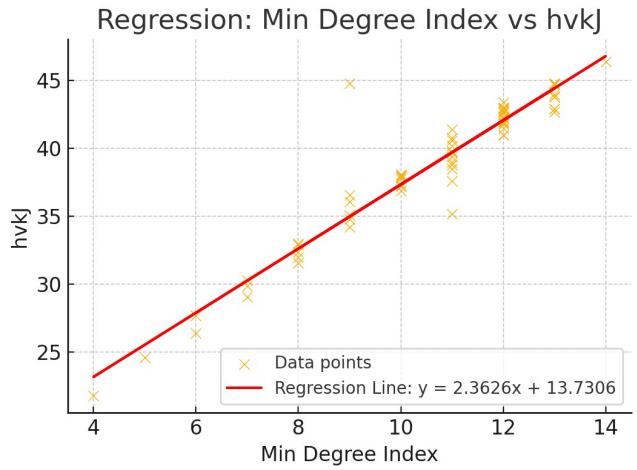


Figure 4: Regression model for hv

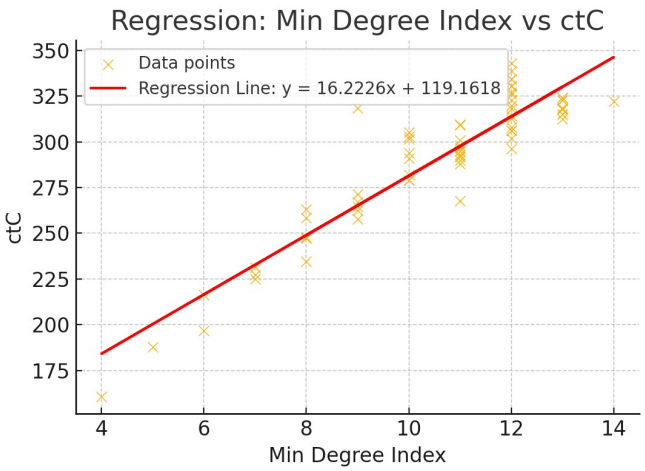


Figure 5: Regression model for ct

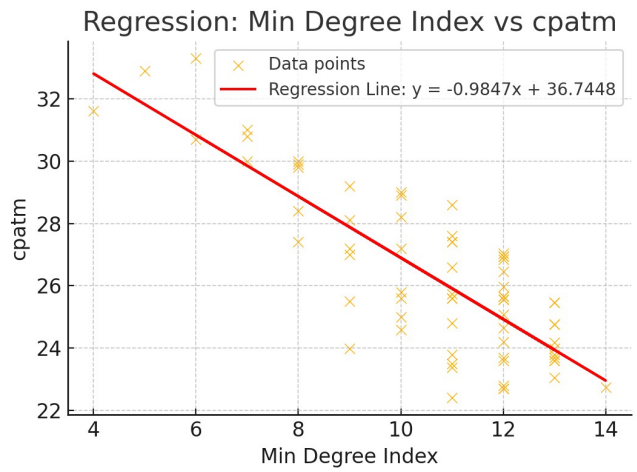


Figure 6: Regression model for cp

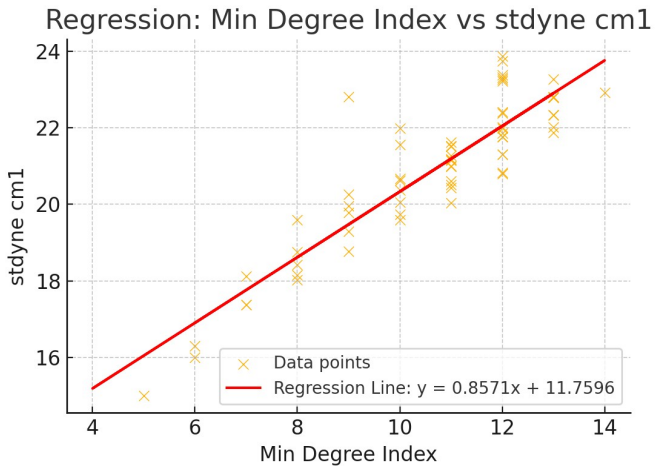


Figure 7: Regression model for st

Conclusion:

Topological indices serve as an important predictive tool for the chemical and physical properties of compounds. The various extended versions of topological indices have become the most interesting aspect of the research due to their extensive applications in the field of chemical sciences. Motivated by the applications, we introduced $MVDI$ and obtained a numerical value of $MVDI$ for some standard and special graphs in terms of their vertices and constants. Further, we obtained $MVDI$ for hexagonal, oxide, silicate and honeycomb networks. We also compared the values of $MVDI$ with the modified elliptic delta index and the elliptic delta index. A QSPR analysis of molecular structures of graphs using $MVDI$ for properties of lower alkanes is done, which shows that, MVDI is strongly correlated with physical properties of lower alkanes.

Conflicts of interest : The authors declare no conflict of interest.

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