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NEW VERTEX-EDGE SOMBOR, NIRMALA AND MISBALANCE INDICES

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Abstract. The molecular structure of a compound contains all the information which would help to determine its chemical, biological, and physical properties. With the help of a theoretical descriptor tool known as topological indices, one can assess these properties. In this paper, we define new vertex-edge degree topological indices namely, the ve-degree Sombor index (SO_{ve}), the ve-degree Nirmala index (N_{ve}), and the ve-degree Misbalance prodeg index (MPI_{ve}). The chemical applicability of those indices have been studied and found good correlation coefficient with different physical/chemical properties of octane isomers. Further, we found the values for the standard graphs and the bounds for SO_{ve} and N_{ve} in terms of MPI_{ve}, $M^{'}_{\beta ve}(G)$, and $F_{ve}(G)$.

Keywords: vertex-edge degree; topological indices.

AMS Subject Classification: 05C07.

1. Introduction

Graph theory played a significant role in molecular chemistry, robotics, physics, networks computer science, statistics, biological activities, and data science. A topological index is a unique number that is mathematically derived from the graph structure. In theoretical chemistry, many such topological indices have been considered, and have more applications in a quantitative structure-property relationship ($QSPR$) and quantitative structure-activity relationship ($QSAR$).
The ($QSPR$)/($QSAR$) studies have an important role in material sciences [1, 2, 3]. The vertex-edge topological indices is a new idea and recently gaining more interest in applied sciences [4, 5, 6, 7, 8, 9, 10, 11, 12]. Let $G = (V, E)$ be a simple connected graph. The number of edges that are incident with the vertex u is known as the degree of the vertex u and is denoted by, $d(u)$. In [5], the set $N(u) = \{u \in V(G) \ : uw \in E(G)\}$ and $N[u] = N(u) \cup \{u\}$ are called as open and closed neighbourhood of the vertex u. The number of different edges that are incident to any vertex from $N[u]$, denoted by $d_{ve}(u)$ and called as ve-degree.

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The first *ve*-degree Zagreb $\alpha(M^1_{\alpha ve})$ index, the first *ve*-degree Zagreb $(M^1_{\beta ve})$ index, the second *ve*-degree Zagreb (M^2_{ve}) index, *ve*-degree Randic (R_{ve}) index, the *ve*-degree atombond connectivity (ABC_{ve})index, the *ve*-degree geometric-arithmetic (GA_{ve}) index, the *ve*-degree harmonic (H_{ve}) index, the *ve*-degree sum-connectivity (χ_{ve}) index, and *ve*-forgotten index are defined as,

$$\sum_{u\in V} d_{ve}(u)^2,\ \sum_{uw\in E}(d_{ve}(u)+d_{ve}(w)),\ \sum_{uw\in E}(d_{ve}(u)\times d_{ve}(w)),\ \sum_{uw\in E}(d_{ve}(u)\times d_{ve}(w))^{-\frac{1}{2}},$$

$$\sum_{uw\in E}\left(\frac{d_{ve}(u)+d_{ve}(w)-2}{d_{ve}(u)\times d_{ve}(w)}\right)^{\frac{1}{2}},\ \sum_{uw\in E}\frac{2\,(d_{ve}(u)\times d_{ve}(w))^{\frac{1}{2}}}{d_{ve}(u)+d_{ve}(w)},\ \sum_{uw\in E}\frac{2}{d_{ve}(u)+d_{ve}(w)},$$

$$\sum_{uw\in E}(d_{ve}(u)+d_{ve}(w))^{-\frac{1}{2}},\ \text{and}\ \sum_{uw\in E}\left(d_{ve}(u)^2+d_{ve}(w)^2\right)$$

respectively. Recently new topological indices have been defined, Sombor index $(SO(G))$ [13], Nirmala index $N(G)$ [14], and Misbalance prodeg index $MPI(G)$ [15].

Some properties of Sombor and Nirmala indices have studied in [15, 16]. In [17, 18] different version of Sombor index is studied and application found in [19]. In [20] the *ve*-degree Sombor index (SO_{ve}) is defined as, $SO_{ve}=\sum_{uw\in E}\sqrt{d_{ve}(u)^2+d_{ve}(w)^2}$. Further, in this paper we define, the *ve*-degree Nirmala index (N_{ve}), and the *ve*-degree Misbalance prodeg index (MPI_{ve}) as follows:

$$N_{ve}=\sum_{uw\in E}\sqrt{d_{ve}(u)+d_{ve}(w)},\ MPI_{ve}=\sum_{uw\in E}\left(\sqrt{d_{ve}(u)}+\sqrt{d_{ve}(w)}\right)$$

respectively. In the next section, we will discuses the chemical applicability of the SO_{ve}, N_{ve}, and MPI_{ve}.

2. Chemical Significance of the SO_{ve}, N_{ve}, and MPI_{ve}

Here, we compute the SO_{ve}, N_{ve}, and MPI_{ve} of octane isomers and molecular graph of octane isomers are shown in Figure 1. We investigate the predictive power of the SO_{ve}, N_{ve}, and MPI_{ve} for certain Physico-chemical properties mainly, acentric factor $(AcenFac)$, entropy (S), enthalpy of vaporization$(HVAP)$, and standard enthalpy of vaporization $(DHVAP)$ of octane isomers. In Table 1, the values of Acentric factor, Entropy,Enthalpy of vaporization (HVAP), Standard enthalpy of vaporization (DHVAP), SO_{ve}, N_{ve}, and MPI_{ve} for octane isomers are tabulated. The correlation between *ve*-degree topological indices and many physicochemical properties of octane isomers is found in Table 2. And it is noted that all indices show a negative strong correlation, therefore these graph invariants are compared with each other by using squares of the correlation coefficients. The graphical representation of the highest values of correlation between *ve*-degree topological indices are shown in Figure 2.

3. Results of SO_{ve}, N_{ve}, and MPI_{ve} on some stranded Graphs.

Here, we found the values of SO_{ve}, N_{ve}, and MPI_{ve} for the particular graph.

Proposition 3.1. *Let $K_{m,n}$ be a complete bipartite graph. Then*

i. $SO_{ve}(K_{m,n})=\sqrt{2}(mn)^2$
ii. $N_{ve}(K_{m,n})=mn\sqrt{2mn}$
iii. $MPI_{ev}(K_{m,n})=2mn\,(\sqrt{mn})$.

Proof. Let $K_{m,n}$ be a complete bipartite graph with $m+n$ vertics and $|V_1|=m$, $|V_2|=n$, $V(K_{m,n})=V_1\cup V_2$. Clearly, every vertex of $v\in V_1$ has mn different edges that incident to any vertex form $N[v]$ and every vertex of $u\in V_2$ has mn different edges that incident to any vertex form $N[u]$.

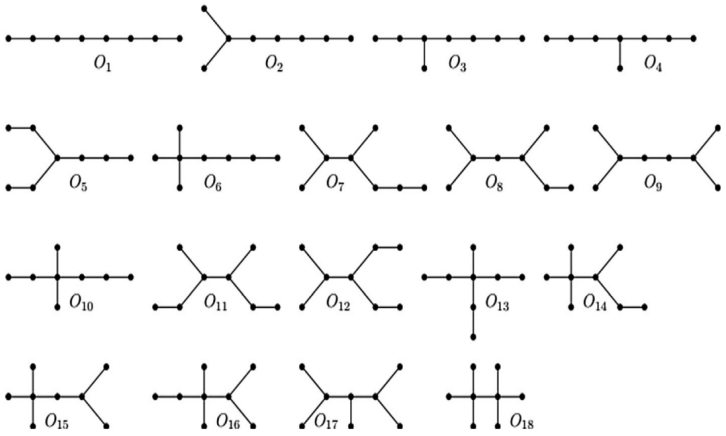

FIGURE 1. Graphs of Octane isomers.

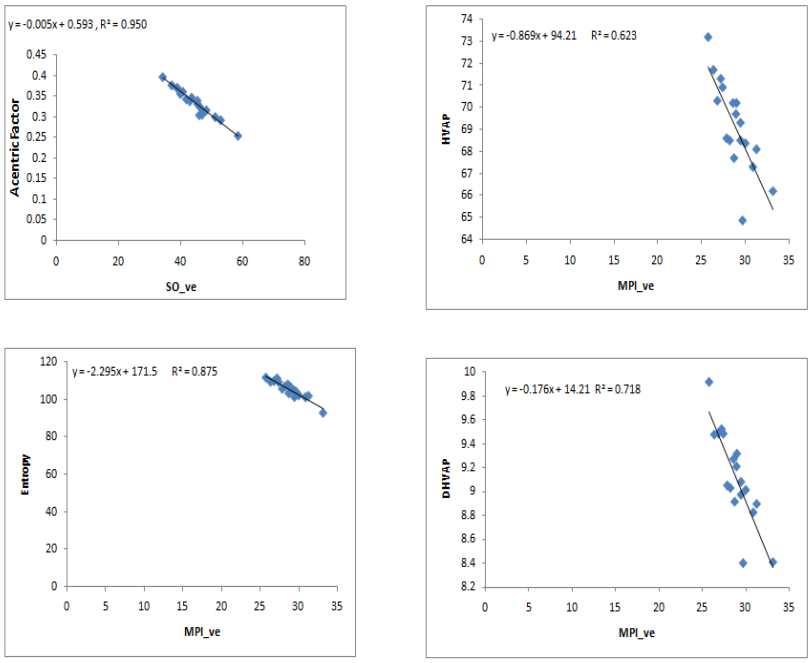

FIGURE 2. Correlation of SO_{ve} with AcenFac, MPI_{ve} with entropy, DHVAP, and HVAP along with their equation of regression.

i.

$$SO_{ve}(K_{m,n}) = \sum_{uw \in E} \sqrt{d_{ve}^2(u) + d_{ve}^2(w)} = \sum_{uw \in E} \sqrt{(mn)^2 + (mn)^2} = \sqrt{2}(mn)^2$$

ii.

$$N_{ve}(K_{m,n}) = \sum_{uw \in E} \sqrt{d_{ve}(u) + d_{ve}(w)} = \sum_{uw \in E} \sqrt{mn + mn} = mn\sqrt{2mn}$$

iii.

$$MPI_{ve}(K_{m,n}) = \sum_{uw \in E} \left(\sqrt{d_{ve}(u)} + \sqrt{d_{ve}(w)}\right) = \sum_{uw \in E} \left(\sqrt{mn} + \sqrt{mn}\right) = 2mn\left(\sqrt{mn}\right).$$

Molecule	*AcenFac*	*Entropy*	*HVAP*	*DHVAP*	SO_{ve}	N_{ve}	MPI_{ve}
2,2,3,3-Tretramethyl-butane	0.255294	93.06	66.2	8.41	58.273	23.641	33.166
2,4-Dimethyl-hexane	0.344223	106.98	68.5	9.029	41.728	20.048	28.218
2-Methyl-heptane	0.377916	109.84	70.3	9.484	37.069	19.594	26.815
2-Methyl-3-ethyl-pentane	0.332433	106.06	69.7	9.209	45.333	20.653	28.938
3-Ethyl-hexane	0.362472	109.43	71.7	9.476	40.613	19.605	26.356
2,2-Dimethyl-hexane	0.339426	103.42	67.7	8.915	42.836	20.361	28.722
3-Methyl-heptane	0.371002	111.26	71.3	9.521	38.786	19.322	27.205
2,3-Dimethyl-hexane	0.348247	108.02	70.2	9.272	43.427	20.355	28.603
2,5-Dimethyl-hexane	0.35683	105.72	68.6	9.051	39.877	19.745	27.872
2,2,4-Trimethyl-pentane	0.30537	104.09	64.87	8.402	45.874	21.072	29.7
4-Methyl-heptane	0.371504	109.32	70.91	9.483	38.846	19.282	27.414
3,3-Dimethyl-hexane	0.322596	104.74	68.5	8.973	46.417	20.987	29.462
3-Methyl-3-ethyl-pentane	0.306899	101.48	69.3	9.081	46.797	21.049	29.457
2,2,3-Trimethyl-pentane	0.300816	101.31	67.3	8.826	51.003	22.021	30.881
3,4-Dimethyl-hexane	0.340345	106.59	70.2	9.316	45.268	21.446	28.989
2,3,3-Trimethyl-pentane	0.293177	102.06	68.1	8.897	52.748	22.349	31.282
Octane	0.397898	111.67	73.19	9.915	34.182	18.249	25.757
2,3,4-Trimethyl-pentane	0.317422	102.39	68.37	9.014	48.144	21.404	30.014

TABLE 1. The values of Acentric factor, Entropy,Enthalpy of vaporization (HVAP), Standard enthalpy of vaporization (DHVAP), SO_{ve}, N_{ve}, and MPI_{ve} for octane isomers.

Index	Acentric Factor	Entropy	HVAP	DHVAP
SO_{ve}	-0.975070878	-0.9213159	-0.715882049	-0.799150905
N_{ve}	-0.959409353	-0.91200543	-0.735557078	-0.803513767
MPI_{ve}	-0.971177506	-0.935705946	-0.789606029	-0.847466686

TABLE 2. The correlation between *ve*-degree topological indices and many physicochemical properties of octane isomers.

□

Corollary 3.1. *Let $K_{n,n}$ be a complete bipartite graph ($n \geq 4$). Then*

i. $SO_{ve}(K_{n,n}) = \sqrt{2}n^4$
ii. $N_{ve}(K_{n,n}) = \sqrt{2}n^3$
iii. $MPI_{ev}(K_{n,n}) = n^3$.

Corollary 3.2. *Let $K_{1,n-1}$ be a star graph ($n \geq 4$). Then*

i. $SO_{ve}(K_{1,n-1}) = \sqrt{2}(n-1)^2$

ii. $N_{ve}(K_{1,n-1}) = (n-1)\sqrt{2(n-1)}$
iii. $MPI_{ev}(K_{1,n-1}) = (n-1)(\sqrt{n-1})$.

Proposition 3.2. *Let C_n be a cycle graph with $n \geq 4$. Then*

i. $SO_{ve}(C_n) = 4n\sqrt{2}$
ii. $N_{ve}(C_n) = 2n\sqrt{2}$
iii. $MPI_{ev}(C_n) = 4n$.

Proof. Let C_n be a cycle graph with $n \geq 4$ vertics. Clearly, every vertex of $v \in V(C_n)$ has 4 different edges that incident to any vertex form $N[v]$.

i.
$$SO_{ve}(C_n) = \sum_{uw \in E} \sqrt{d_{ve}^2(u) + d_{ve}^2(w)} = \sum_{uw \in E} \sqrt{4^2 + 4^2} = 4n\sqrt{2}$$

ii.
$$N_{ve}(C_n) = \sum_{uw \in E} \sqrt{d_{ve}(u) + d_{ve}(w)} = \sum_{uw \in E} \sqrt{4 + 4} = 2n\sqrt{2}$$

iii.
$$MPI_{ve}(C_n) = \sum_{uw \in E} \left(\sqrt{d_{ve}(u)} + \sqrt{d_{ve}(w)}\right) = \sum_{uw \in E} \left(\sqrt{4} + \sqrt{4}\right) = 4n$$

□

Proposition 3.3. *Let K_n be a complete graph with $n(\geq 4)$ vertics. Then*

i. $SO_{ve}(K_n) = \dfrac{n^2(n-1)^2}{2\sqrt{2}}$
ii. $N_{ve}(K_n) = \dfrac{(n(n-1))^{3/2}}{2}$
iii. $MPI_{ev}(K_n) = \dfrac{(n(n-1))^{3/2}}{\sqrt{2}}$.

Proof. Let K_n be a complete graph with n vertics. Clearly, every vertex of $v \in V(k_n)$ has $n(n-1)/2$ different edges that incident to any vertex form $N[v]$.

i.
$$SO_{ve}(K_n) = \sum_{uw \in E} \sqrt{d_{ve}^2(u) + d_{ve}^2(w)} = \sum_{uw \in E} \sqrt{[n(n-1)/2]^2 + [n(n-1)/2]^2} = \frac{n^2(n-1)^2}{2\sqrt{2}}$$

ii.
$$N_{ve}(K_n) = \sum_{uw \in E} \sqrt{d_{ve}(u) + d_{ve}(w)} = \sum_{uw \in E} \sqrt{[n(n-1)/2] + [n(n-1)/2]} = \frac{(n(n-1))^{3/2}}{2}$$

iii.
$$\begin{aligned} MPI_{ve}(K_n) &= \sum_{uw \in E} \left(\sqrt{d_{ve}(u)} + \sqrt{d_{ve}(w)}\right) = \sum_{uw \in E} \left(\sqrt{[n(n-1)/2]} + \sqrt{[n(n-1)/2]}\right) \\ &= \frac{(n(n-1))^{3/2}}{\sqrt{2}} \end{aligned}$$

□

Proposition 3.4. *For the path graph $P_n (n \geq 5)$, $d_{ve}(v_1) = d_{ve}(v_n) = 2$, $d_{ve}(v_2) = d_{ve}(v_{n-1}) = 3$, and remaining vertices has the ve-degree 4. Then,*

i.
$$SO_{ve}(P_n) = 2\sqrt{13}(n-1) + 10(n-1) + 4\sqrt{2}(n-1)(n-5)$$

ii.
$$N_{ve}(P_n) = 2\sqrt{5}(n-1) + 2(n-1)\sqrt{7} + 2\sqrt{2}(n-1)(n-5)$$

iii.

$$MPI_{ve}(P_n) = (n-1)[2\sqrt{2} + 4\sqrt{3} + 4(n-5) + 4].$$

Proof. With the definitions and *ve*-degree of each vertex one can easily arrive the results. □

4. Bounds

In this section, we found the bounds for SO_{ve} and N_{ve} in terms of MPI_{ve}, $M'_{\beta ve}(G)$, and $F_{ve}(G)$.

Lemma 4.1. *For any positive numbers α and β,*

$$\frac{1}{\sqrt{2}}(\alpha + \beta) \leq \sqrt{\alpha^2 + \beta^2} \leq \alpha + \beta.$$

Equality on the left-hand side holds if and only if $\alpha = \beta$.

Theorem 4.1. *For any non-trivial connected graph G,*

$$\frac{1}{\sqrt{2}} M'_{\beta ve}(G) \leq SO_{ve}(G) \leq M'_{\beta ve}(G).$$

Proof. With help of definitions and lemma 4.1, we arrive the result. □

Lemma 4.2. *Let α and β be any non-negetive real numbers. Then*

$$\sqrt{\alpha + \beta} \geq \frac{1}{\sqrt{2}} \left(\sqrt{\alpha} + \sqrt{\beta} \right).$$

Theorem 4.2. *Let G be a connected graph of order n and size m. Then*

$$\frac{1}{\sqrt{2}} MPI_{ve}(G) \leq N_{ve}(G) \leq MPI_{ve}(G).$$

Proof. If $\alpha = d_{ve}(u)$ and $\beta = d_{ve}(w)$ in Lemma 4.2, then we get

$$\sqrt{d_{ve}(u) + d_{ve}(w)} \geq \frac{1}{\sqrt{2}} \left(\sqrt{d_{ve}(u)} + \sqrt{d_{ve}(w)} \right)$$

By the definition of *ve*-Nirmala index, we have

$$N_{ve}(G) = \sum_{uw \in E} \sqrt{d_{ve}(u) + d_{ve}(w)} \geq \frac{1}{\sqrt{2}} \sum_{uw \in E} \left(\sqrt{d_{ve}(u)} + \sqrt{d_{ve}(w)} \right) = \frac{1}{\sqrt{2}} MPI_{ve}(G)$$

By the definition of *ve*-Nirmala index, we have

$$\begin{aligned} N_{ve}(G) &= \sum_{uw \in E} \sqrt{d_{ve}(u) + d_{ve}(w)} \\ &= \sum_{uw \in E} \left[\left(\sqrt{d_{ve}(u)} + \sqrt{d_{ve}(w)} \right)^2 - 2\sqrt{d_{ve}(u) d_{ve}(w)} \right]^{1/2} \\ &\leq \sum_{uw \in E} \left(\sqrt{d_{ve}(u)} + \sqrt{d_{ve}(w)} \right) = MPI_{ve}(G) \end{aligned}$$

□

Theorem 4.3. *Let G be a connected graph with m edges. Then*

$$SO_{ve}(G) \leq \sqrt{m F_{ve}(G)}.$$

Proof. Using the Cauchy-Schwarz inequity, we get

$$\left(\sum_{uw \in E} d_{ve}(u)^2 + d_{ve}(w)^2 \right)^2 \leq \sum_{uw \in E} 1 \sum_{uw \in E} \left(d_{ve}(u)^2 + d_{ve}(w)^2 \right) = m F_{ve}(G)$$

□

Conclusion

In this study, we have computed SO_{ve}, N_{ve}, and MPI_{ve} for Standard graphs, and found the bounds for SO_{ve} and N_{ve} in terms of MPI_{ve}, $M'_{\beta ve}(G)$, and $F_{ve}(G)$. The predictive ability of the ve-degree index is greater and also has a better correlation than classic degree-based indices. Also, the predictive ability of newly defined ve-degree indices has been tested on some physicochemical properties of octanes.

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