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Generalized Reciprocal Sanskruti Index: Chemical Applicability and Bounds

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Abstract: In this paper, we put forward the generalization of reciprocal Sanskruti index $\mathcal{RS}^{\alpha}$ for some $\alpha \in Z^{+}$. *For* $\alpha = 3$ the prediction potentiality of $\mathcal{RS}^{3}$ is discussed with the physicochemical properties of the set of octane isomers. And also we study the mathematical properties of $\mathcal{RS}^{3}$.

Keywords: Topological indices; Sanskruti index; Reciprocal Sanskruti index.

1. Introduction

Let $G = (V, E)$ be a simple graph with $|V| = n$ and $|E| = m$. Let $\Delta = \deg(v_1) \geq \deg(v_2) \geq \deg(v_3), \ldots, \geq \deg(v_n) = \delta$ be vertex degree sequence and let $\Delta' = \sigma(v_1) \geq \sigma(v_2) \geq \sigma(v_3) \geq, \ldots, \sigma(v_n) = \delta'$ *be neighborhood degree* sequence of G respectively. Where $\sigma(u) = \sum_{v \epsilon N(u)} \deg(v)$ and $N(u) = \{v \backslash uv \in E(G)\}$. S(G) and L(G) denote the subdivision and line graph of G, respectively.

A Topological Index of a graph is a numerical value that is invariant under the automorphism of graphs. Due to numerous applications in chemistry as a molecular structure descriptors, topological indices gained considerable popularity in the field of mathematical chemistry. These topological indices are used in QSAR/QSPR [1, 4, 12, 16, 17] studies to predict the physicochemical characteristics and biological activities of chemical compounds using a molecular graph. Topological indices can be classified into several distinct categories. One of the widely used group is the so-called degree-based topological indices. A large number of degree-based topological indices have been studied so far [2-10,13-15,18], and references are cited therein.

The most studied topological indices are the Zagreb indices.

$$M_1(G) = \sum_{v \sim u} d_G(v)^2 \quad (1)$$

$$M_2(G) = \sum_{v \sim u} d_G(v) d_G(u) \quad (2)$$

The Sanskruti index [11] is defined as

$$S(G) = \sum_{v_i \sim v_j} \left(\frac{v_i v_j}{v_i + v_j - 2}\right)^3 \quad (3)$$

Motivated by the previous research on Sanskruti index, here we propose the following topological indices:

- Generalized Reciprocal Sanskruti Index:

$$\mathcal{RS}(G)^{\propto} = \sum_{v_i \sim v_j} \left(\frac{v_{i+}v_j-2}{v_i v_j}\right)^{\propto} \quad (4)$$

- For $\propto = 1$,

$$\mathcal{RS}(\text{G}) = \sum_{v_i \sim v_j} \left(\frac{v_{i+}v_j-2}{v_i v_j}\right) \quad (5)$$

- Randic type reciprocal Sanskruti index:

$$RT = \sum_{v_i \sim v_j} \frac{1}{v_i v_j} \quad (6)$$

- Reduced Sanskruti index:

$$RSI = \sum_{v_i \sim v_j} \frac{v_{i+}v_j}{v_i v_j} \quad (7)$$

In this paper we are intrested to work on the reciprocal sanskruti index for $\propto = 3$. Which is defined as follows:

$$\mathcal{RS}(G)^3 = \sum_{v_i \sim v_j} \left(\frac{v_{i+}v_j-2}{v_i v_j}\right)^3 \quad (8)$$

Whenever we introduced a new topological index, it is mandatory to check its applicability in chemistry as a molecular structure descriptor. Therefore, in the following section, we investigate the applicability of $\mathcal{RS}(G)^3$ index.

2. Materials and Methods

2.1. On chemical applicability of the RS(G)^3-Index.

Here we have examined the chemical applicability of the reciprocal Sanskruti $\mathcal{RS}(G)^3 -$ index and compared the values with the Sanskruti $\mathcal{S}(G) -$ index for modeling the physical and chemical properties [boiling points(BP), molar volumes (mv) at 20°C, molar refractions (mr) at 20°C, heats of vaporization (hv) at 25°C, surface tensions (st) 20°C and melting points (mp), acentric factor (AcentFac), and DHVAP] of octane isomers. The $\mathcal{RS}(G)^3$ was tested using a data set of octane isomers found at (http://www.moleculardescriptors.eu//dataset.htm). The values are compiled in Table 1.

Table 1. Physico-chemical properties of octane isomers.

Alkane	AF	DHVAP	BP	TC	PC	S	D	R_m^2	$-\Delta H_f$	$-\Delta H_v$
n-octane	0.3978	9.915	125.70	296.20	24.64	111.67	0.7025	2.0449	208.6	41.49
2M	0.3779	9.484	117.6	288.0	24.80	109.84	0.6980	1.8913	215.4	39.67
3M	0.3710	9.521	118.9	292.0	25.60	111.26	0.7058	1.7984	212.5	39.83
4M	0.3715	9.483	117.7	290.0	25.60	109.32	0.7046	1.7673	210.7	39.64
3E	0.3624	9.476	118.5	292.0	25.74	109.43	0.7136	1.7673	210.7	39.64
22MM	0.3394	8.915	106.8	279.0	25.60	103.42	0.6953	1.6744	224.6	37.28
23MM	0.3482	9.272	115.6	293.0	26.60	108.02	0.7121	1.6464	213.8	38.78
24MM	0.3442	9.029	109.4	282.0	25.80	106.98	0.7004	1.6142	219.2	37.76
25MM	0.3568	9.051	109.1	279.0	25.00	105.72	0.6935	1.6449	222.5	37.85
33MM	0.3225	8.973	112.0	290.8	27.20	104.74	0.7100	1.7377	220.0	37.53
34MM	0.3403	9.316	117.7	298.0	27.40	106.59	0.7200	1.5230	212.8	38.97
2M3E	0.3324	9.209	115.6	295.0	27.40	106.06	0.7193	1.5525	211.0	38.52
3M3E	0.3068	9.081	118.3	305.0	28.90	101.48	0.7274	1.5212	214.8	37.99
223MMM	0.3008	8.826	109.8	294.0	28.20	101.31	0.7161	1.4306	220.0	36.91
224MMM	0.3053	8.402	99.24	271.1	25.50	104.09	0.6919	1.4010	224.0	35.14
233MM	0.2931	8.897	114.8	303.0	29.00	102.06	0.7262	1.4931	216.3	37.27
234MMM	0.3174	9.014	113.5	295.0	27.60	102.39	0.7191	1.3698	217.3	37.75
2233MMMM	0.2552	8.41	106.5	270.8	24.50	93.06	0.8242	1.4612	225.6	42.90

Surprisingly, we can see that the correlation coefficient value of $\mathcal{RS}(G)^3$ for the boiling points of octane, the isomer is $r = 0.701$, whereas for $\mathcal{S}(G)$ the correlation coefficient value is $r = 0.366$. Similarly for other physical properties of octane isomers such as heats, critical

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temperature, critical pressure, density, entropy and mean radius, the correlation coefficient value for $\mathcal{RS}(G)^3$ is $r = 0.670$, 0.473, 0.636, 0.810 and 0.687 respectively, where as for $\mathcal{S}(G)$ the correlation coefficient value is $r = 0.435$, 0.010, 0.611, 0.857 and 0.669 respectively. Clearly, the reciprocal Sanskruti index $\mathcal{RS}(G)^3$ shows a better correlation than $\mathcal{S}(G)$. In Figure 1, the correlation coefficient of $\mathcal{RS}(G)^3$ and S(G) are depicted.

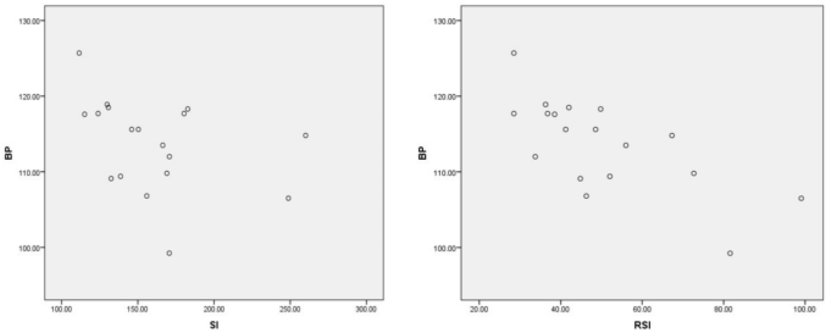

Figure 1. Correlation coefficient.

3. Results and Discussion

3.1. Mathematical properties of $\mathcal{RS}(G)^3$.

Since, $(\frac{v_{i+}v_j-2}{v_iv_j})^3$ is equal for all edges if a graph G is regular or biregular. Therefore we have the following axillary results:

Proposition 1. For any r-regular graph G, $S^3(G) = \frac{4n(r^2-1)^3}{r^{11}}$

Proof. Let G be a r-regular graph. Then for every $v \in V(G), v_j = r^2$. Further, every r-regular graph containing $\frac{nr}{2}$ edges. Therefore we have,

$$\mathcal{RS}(G)^3 = \sum_{v_i \sim v_j} \left(\frac{v_{i+}v_j - 2}{v_iv_j}\right)^3$$

$$= \frac{nr}{2}(\frac{r^2+r^2-2}{r^4})^3$$

$$= \frac{4n((n-1)^2-1)^3}{r^{11}}$$

Proposition 2.

(a) For a complete graph K_n, $S^3(K_n) = \frac{4n((n-1)^2-1)^3}{(n-1)^{11}}$

(b) For cycle graph C_n, $S^3(C_n) = \frac{27n}{512}$

(c) For path graph P_n, $S^3(P_n) = \frac{27n+47}{512}$

(d) For the wheel graph W_n, $S^3(W_n) = (n-1)[\left(\frac{4n-6}{3(n-1)^2}\right)^3 + \left(\frac{n+8}{n+5}\right)^3]$

(e) For complete biparatite graph $K_{r,s}; 2 \leq r < s, S^3(K_{r,s}) = \frac{8(rs-1)^3}{rs^5}$

Proof. (a) and (b) follows by Proposition 1, putting r = n-1 and r =2 respectively.
(c) Let V(P_n)={v_1, v_2, $v_{3,......,}v_n$} where v_1 and v_n are pendent vertices of P_n. Then for every $v \in V\{v_1, v_n\}, v_j = 4$ and $\sigma(v_1) = 5 = \sigma(v_n)$. Since $E(P_n) = n-1$, therefore, we have

$$\mathcal{RS}(P_n)^3 = \sum_{v_i \sim v_j} (\frac{v_i + v_j - 2}{v_i v_j})^3$$
$$= \text{(n-3)}\left(\frac{4+4-2}{4^2}\right)^3 + 2\left(\frac{2+3-2}{2\times 3}\right)^3$$
$$= \frac{27n+47}{512}$$

(d) Let $V(W_n)=\{v_1, v_2, v_3,\ldots,v_n\}$where v_1 is a central vertex of W_n. Then for every $v \in V\backslash\{v_1\}, v_j = n+5 \ and\ \sigma(v_1) = 3(n-1)$. Since $E(W_n) = 2(n-1)$, therefore, we have

$$\mathcal{RS}(W_n)^3 = \sum_{v_i \sim v_j} (\frac{v_i + v_j - 2}{v_i v_j})^3$$
$$=(n-1)\left(\frac{3(n-1)+(n-1)-2}{3(n-1)^2}\right)^3 + (n-1)\left(\frac{(n+5)+(n+5)-2}{(n+5)^2}\right)^3$$
$$=\text{(n-1)}[\left(\frac{4n-6}{3(n-1)^2}\right)^3 \left(\frac{n+8}{n+5}\right)^3]$$

(e) Let $V(K_{r,s}) = v_1 \cup v_2$ where $v_1 = \{v_1, v_2, v_3, \ldots, v_r\}$ and $v_2 = \{v_{r+1}, v_{r+2}, v_{r+3}, \ldots, v_s\}$. Clearly, every $v \in v_1, v_j = rs$ and $u \in v_2, v_i = sr$. Since $E(K_{r,s}) = rs$
therefore, we have

$$\mathcal{RS}(K_{r,s})^3 = \sum_{v_i \sim v_j} (\frac{v_i + v_j - 2}{v_i v_j})^3$$
$$= rs\left(\frac{rs+sr-2)}{rs^2}\right)^3$$
$$= \frac{8(rs-1)^3}{rs^5}$$

We need the following well-known results to obtain bounds for $RS(G)^3$.

Lemma 1 ([19]). Let a_i, i = 1,2,3,…,m be a positive real number sequence. Then for any real $r, r \geq 1\ or\ r \leq 0$, the following inequality holds

$\sum_{i=1}^{m} a_i^r \geq m^{1-r}(\sum_{i=1}^{m} a_i)$. (9)

Equality holds if and only if $a_1 = a_2 = \cdots = a_m$.

Lemma 2 ([20]). Let a_i and b_i, i=1,2,3,…,m be a positive real number sequences. Then for any real $r \geq 0$ the following inequality holds

$\sum_{i=1}^{m} \frac{a_i^{r+1}}{b_i^r} \geq \frac{(\sum_{i=1}^{m} a_i)^{r+1}}{(\sum_{i=1}^{m} b_i)^r}$ (10)

Equality holds if and only if $\frac{a_1}{b_1} = \frac{a_2}{b_2} = \cdots = \frac{a_m}{b_m}$.

3.2. Bounds for $RS(G)^3$.

Next, we have the following lower bound for $RS(G)^3$ in terms of maximum degree and the size of a graph G.

Theorem 3. For any graph G without isolated vertices,

$RS(G)^3 \geq 8m(\frac{1}{\Delta^2} - \frac{1}{\Delta^4})^3$ (11)

Proof. Let G be graph without isolated vertices of size m and maximum degree Δ. Since for any $v \in V, v_j \leq \Delta^2$. Therefore, we have,

$$RS(G)^3 = \sum_{v_i \sim v_j} (\frac{v_i + v_j - 2}{v_i v_j})^3 \geq m\left(\frac{\Delta^2 + \Delta^2 - 2}{\Delta^4}\right)^3$$

$$= 8m\left(\frac{\Delta^2 - 1}{\Delta^4}\right)^3$$

$$=8m\left(\frac{1}{\Delta^2} - \frac{1}{\Delta^4}\right)^3$$

In the following results, we obtain lower bound for $RS(G)^3$ in terms of maximum degree Δ.

Theorem 4. For any n-vertex graph G and maximum degree Δ,we have

$$RS(G)^3 \geq \frac{8\left(\Delta^4-1\right)^3}{\Delta^{12}(\Delta^2+1)^3} \quad (12)$$

Proof. Let G be a n-vertex graph with a maximum degree Δ, we have

$$\mathcal{RS}(G)^3 = \sum_{v_i \sim v_j} \left(\frac{v_{i+}v_j-2}{v_i v_j}\right)^3 \quad (13)$$

$$= \sum_{v_i \sim v_j} \left(\frac{v_i v_j-1}{v_i v_j}\right)^3 \left(\frac{v_{i+}v_j-2}{v_i v_j-1}\right)^3 \quad (14)$$

Since $\left(v_i - v_j\right)^2 \geq 0$, therefore it is easy to check that

$$\frac{v_{i+}v_j-2}{v_i v_j-1} = \frac{1}{v_i+1} + \frac{1}{v_j+1}. \quad (15)$$

Since $v_i \leq \Delta^2$ therefore (15) becomes

$$\frac{v_{i+}v_j-2}{v_i v_j-1} = \frac{1}{\Delta^2+1} + \frac{1}{\Delta^2+1} \quad (16)$$

Employing (16) in (14), we get

$$RS(G)^3 \geq \left(\frac{\Delta^2\Delta^2 - 1}{\Delta^4}\right)^3 \left(\frac{2}{\Delta^2 + 1}\right)^3$$

$$= \frac{8(\Delta^4 - 1)^3}{\Delta^{12}(\Delta^2 + 1)^3}$$

Theorem 5. Let G be a graph without isolated vertex. Then

$$RS(G)^3 \geq \frac{(RSI - 2RT)^3}{m^2}$$

Proof. Let G be a graph without isolated vertex. Then set $r = 3, a_i = \frac{v_{i+}v_j-2}{v_i v_j}$ where the summation is performed over all edges of G then (9) is transformed into

$$\sum_{v_i \sim v_j} \left(\frac{v_{i+}v_j - 2}{v_i v_j}\right)^3 \geq m^{1-3} \sum_{v_i \sim v_j} \left(\frac{v_{i+}v_j - 2}{v_i v_j}\right)^3$$

$$\geq \left(\sum_{v_i \sim v_j} \frac{v_{i+}v_j}{v_i v_j} - \sum_{v_i \sim v_j} \frac{2}{v_i v_j}\right)^3$$

$$= \frac{(RSI-2RT)^3}{m^2}$$

Theorem 6. Let G be a graph without isolated vertex with size at least 2. Then

$$RS(G)^3 \leq (2M_2 - 2m)^3 (RT)^3$$

Proof. Observe that the following identity holds

$$2M_2 - 2m = \sum_{v_i \sim v_j} (v_{i+}v_j) - 2m$$

$$=\sum_{v_i \sim v_j} v_{i+}v_j - 2$$

$$(2M_2 - 2m)^3 = \sum_{v_i \sim v_j} \frac{\left(\frac{v_{i+}v_j - 2}{v_i v_j}\right)^3}{\left(\frac{1}{v_i v_j}\right)^3}$$

Set $r = 2,\ a_i = \frac{v_{i+}v_j - 2}{v_i v_j}$ and $b_i = \frac{1}{v_i v_j}$ in (10), we get

$$\sum_{v_i \sim v_j} \frac{\left(\frac{v_{i+}v_j - 2}{v_i v_j}\right)^3}{\left(\frac{1}{v_i v_j}\right)^3} \times \frac{1}{v_i v_j} \geq \frac{\left(\sum_{v_i \sim v_j}\left(\frac{1}{v_i v_j}\right)\right)^3}{\left(\sum_{v_i \sim v_j} \frac{1}{v_i v_j}\right)^2}$$

$$(2M_2 - 2m)^3 RT \geq \frac{RS(G)^3}{(RT)^{\epsilon}}$$

$$RS(G)^3 \leq (2M_2 - 2m)^3 (RT)^3.$$

4. Conclusions

Inspired by the work on the Sanskruti index, the reciprocal Sanskruti index is proposed. The value of the reciprocal Sanskruti index is calculated for octane isomers. The chemical applicability is compared to model the physical and chemical properties of octane isomers. The reciprocal Sanskruti index gives better results than the Sanskruti index.

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Conflicts of Interest

The authors declare no conflict of interest.

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