

Novel Sombor-Index-Like Topological Indices with Geometry and Calculus

Mert Sinan Öz

Abstract: Gutman designed the Sombor index (SO) based on a geometric approach in [4] and subsequently developed six SO -like vertex-degree-based (VDB) topological indices in conjunction with this approach in [5]. Within this framework, we propose five novel SO -like VDB topological indices based on geometry and calculus. We recall that two of the proposed indices are related to the elliptic Sombor index (ESO) and also highlight the relationship between two of the proposed indices and the second Gourava index (GO_2). Afterward, we investigate the chemical usefulness of the four proposed indices and observe that two of them have better chemical applicability potential compared to the others. Moreover, we compare the obtained results with those obtained for ESO and GO_2 . Furthermore, we determine connected graphs and trees attaining the extremal values for the two proposed indices among all connected graphs and trees, respectively. Lastly, we present the relationships between the two proposed indices and SO from a mathematical perspective.

Keywords: the Sombor index, the Sombor-index-like indices, vertex-degree-based indices.

1 Introduction

A graph without any weighted, directed or multiple edges, and without any loops is called a simple graph. In this paper, we assume that all graphs are simple. Let $G = (V, E)$ be such a graph with vertex set V and edge set E . Let d_u , uv and Δ denote the degree of the vertex $u \in V$, the edge $uv \in E$ connecting the vertices $u, v \in V$ and the maximum degree of the vertex in G , respectively.

Topological indices have been widely studied, especially in the prediction of physico-chemical and biological activities of chemical compounds in QSAR and QSPR analyses [3, 8, 12]. Although there are various types of topological indices, one of the most studied types is the VDB topological index type.

A vertex-degree-based topological index of G is expressed as the sum of a function whose variables are the end vertices degrees of the edges, where the summation is over all edges of G .

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Mert Sinan Öz (ORCID 0000-0002-6206-0362) is with the Bursa Technical University, Faculty of Engineering and Natural Sciences, Department of Mathematics, Bursa, Turkey, sinan.oz@btu.edu.tr

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In [4], the Sombor index was introduced by Gutman by carrying the end vertices degrees of the edges to the 2D-coordinate plane and is expressed as follows:

$$SO(G) = \sum_{uv \in E} \sqrt{d_u^2 + d_v^2}.$$

This idea was clearly illustrated in Fig. 1 presented in [5]. Thanks to this idea geometric interpretations of many well-known VDB topological indices and six new SO-like VDB topological indices based on a geometric approach were presented in [5].

Furthermore, the notation presented in Fig. 1 led to the emergence of the elliptic Sombor index [6] based on the geometric approach as follows:

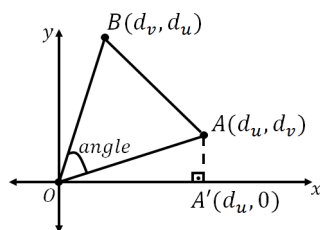
$$ESO(G) = \sum_{uv \in E} (d_u + d_v) \sqrt{d_u^2 + d_v^2}.$$

Moreover, the Gourava index was defined in [9] as follows:

$$GO_2(G) = \sum_{uv \in E} (d_u + d_v) d_u d_v.$$

Since the area of the triangle AOA' presented in Fig. 1 is equal to $\frac{1}{2}d_u d_v$, it can be interpreted geometrically that the volume of the triangular prism whose base is the triangle AOA' and whose height is $(d_u + d_v)$ induces GO_2 .

Fig. 1. A geometric representation of an edge uv of G , where $d_u > d_v$. The points A and B represent the degree-point of the edge uv and the respective dual of the edge uv .

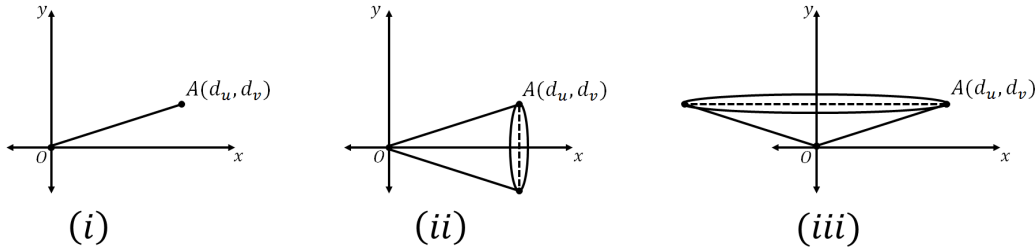


In the second section, five new SO-like graph indices based on geometry and calculus are proposed. In the third section, the chemical applicability potentials of four of the proposed indices are investigated in the context of structure sensitivity (*SS*), abruptness (*Abr*), degeneracy, and correlation coefficients with several thermodynamic properties of octane isomers. Moreover, the obtained results are compared with the results obtained for *ESO* and *GO*₂, which are related to two of the proposed indices. As a result of these investigations, it is observed that two indices have better chemical applicability potential among the four proposed indices. In the last section, connected graphs and trees attaining the extremal values are determined for the two proposed indices, which have the potential for better chemical applicability, among all connected graphs and trees, respectively.

2 Novel SO-like VDB topological indices

Let us consider the representation of an edge of G in Fig. 2 (i) by focusing on the degree-point A and ignoring the dual-degree-point. If we rotate the line segment $\overline{OA}$ which is a curve with the formula $y = f(x) = \frac{d_v}{d_u}x$ around the x -axis and y -axis, then we get a 3D-cone as shown in Fig. 2 (ii) and (iii), respectively.

Fig. 2. (i) A geometric representation of an edge uv of G without the respective dual-degree-point, where $d_u > d_v$. (ii) The 3D-cone (*cone1*) obtained after rotation around the x -axis. (iii) The 3D-cone (*cone2*) obtained after rotation around the y -axis.



In [6], it is mentioned that the surface areas of the *cone1* and *cone2* are equal to

$$S_{cone1} = \pi \cdot d_v \sqrt{d_u^2 + d_v^2} \text{ and } S_{cone2} = \pi \cdot d_u \sqrt{d_u^2 + d_v^2}, \text{ respectively.}$$

In the same paper, it is also stated that the sum of $S_{cone1} + S_{cone2}$ is another way to reveal the ESO by ignoring constants.

Here, we focus on computing the volumes of *cone1* and *cone2* with the help of the integral as follows:

$$V_{cone1} = \pi \int_0^{d_u} \left(\frac{d_v}{d_u} x \right)^2 dx = \pi \frac{d_v^2}{d_u^2} \int_0^{d_u} x^2 dx = \pi \frac{d_v^2}{d_u^2} \left(\frac{x^3}{3} \Big|_0^{d_u} \right) = \pi \frac{d_v^2}{d_u^2} \frac{d_u^3}{3} = \frac{\pi}{3} d_u \cdot d_v^2.$$

$$V_{cone2} = \pi \int_0^{d_v} \left(\frac{d_u}{d_v} y \right)^2 dy = \pi \frac{d_u^2}{d_v^2} \int_0^{d_v} y^2 dy = \pi \frac{d_u^2}{d_v^2} \left(\frac{y^3}{3} \Big|_0^{d_v} \right) = \pi \frac{d_u^2}{d_v^2} \frac{d_v^3}{3} = \frac{\pi}{3} d_v \cdot d_u^2.$$

Hence, one can observe that the sum of $V_{cone1} + V_{cone2}$ leads to the GO_2 by ignoring constants.

Finally, another 3D-shape (solid object) is obtained by rotating the total area of the triangle AOB shown in Fig. 1 around the x -axis (or y -axis). Similarly, the volume of this solid object can be computed with the help of the integral by dividing the total area into two pieces as follows:

Before starting the operations, it should be noted that the line segment $\overline{OA}$ has the formula $y = f(x) = \frac{d_v}{d_u}x$, the line segment $\overline{OB}$ has the formula $y = f(x) = \frac{d_u}{d_v}x$ and the line segment $\overline{AB}$ has the formula $y = f(x) = -x + d_u + d_v$.

$$\begin{aligned} V_{solid} &= \pi \int_0^{d_v} \left[\left(\frac{d_u}{d_v}x \right)^2 - \left(\frac{d_v}{d_u}x \right)^2 \right] dx + \pi \int_{d_v}^{d_u} \left[(-x + d_u + d_v)^2 - \left(\frac{d_v}{d_u}x \right)^2 \right] dx \\ &= \frac{\pi}{3} [d_u^2 \cdot d_v - d_u \cdot d_v^2 + d_u^3 - d_v^3]. \end{aligned}$$

Moreover, it can be observed that the same result is obtained for these curves when rotated around the y -axis. As a result, we can propose the following five new SO-like graph indices induced by the formulae above.

Definition 2.1. (*x-Line Volume Index*) Let $G = (V, E)$ be a graph and let $d_u \geq d_v$.

$$SO_7(G) = \sum_{uv \in E} d_u \cdot d_v^2.$$

Definition 2.2. (*y-Line Volume Index*) Let $G = (V, E)$ be a graph and let $d_u \geq d_v$.

$$SO_8(G) = \sum_{uv \in E} d_u^2 \cdot d_v.$$

Definition 2.3. (*x-Surface Area Index*) Let $G = (V, E)$ be a graph and let $d_u \geq d_v$.

$$SO_9(G) = \sum_{uv \in E} d_v \sqrt{d_u^2 + d_v^2}.$$

Definition 2.4. (*y-Surface Area Index*) Let $G = (V, E)$ be a graph and let $d_u \geq d_v$.

$$SO_{10}(G) = \sum_{uv \in E} d_u \sqrt{d_u^2 + d_v^2}.$$

Definition 2.5. (*Triangle Volume Index*) Let $G = (V, E)$ be a graph and let $d_u \geq d_v$.

$$SO_{11}(G) = \sum_{uv \in E} [d_u^2 \cdot d_v - d_u \cdot d_v^2 + d_u^3 - d_v^3].$$

3 Chemical applicability potential

The absolute values of the correlation coefficient values ($|R|$) between the thermodynamic properties of octane isomers such as boiling point (B. P.), acentric factor (AcenFac), standard enthalpy of vaporization (DHVAP), entropy, enthalpy of vaporization (HVAP) and enthalpy of formation and stated topological indices are given in Table 1.

Table 1. The absolute values of the correlation coefficients ($|R|$) between the indices and stated chemical properties of octane isomers.

	ESO	GO_2	SO_7	SO_8	SO_9	SO_{10}
B. P.	0,67740	0,48394	0,15385	0,58534	0,25226	0,72857
AcenFac	0,97435	0,98206	0,80059	0,98483	0,85811	0,95718
DHVAP	0,91660	0,80561	0,50622	0,87045	0,59707	0,93897
Entropy	0,95756	0,95024	0,79697	0,94364	0,85736	0,93811
HVAP	0,85997	0,71991	0,40034	0,79949	0,50194	0,89163
Enthalpy	0,74407	0,55928	0,23704	0,65184	0,34181	0,78842

It can be seen from Table 1 that SO_8 and SO_{10} have the highest and second highest $|R|$ values among the proposed SO-like topological indices. However, it is also observed that SO_{10} has higher $|R|$ values than SO_8 for all properties except the acentric factor and entropy. It is also observed that the $|R|$ values of SO_8 are slightly higher than the $|R|$ values of its related index GO_2 , except for entropy, while SO_{10} has close $|R|$ values with its related index ESO .

In Table 2, both structure sensitivity (SS) and abruptness (Abr) values, including $\frac{SS}{Abr}$ values for ESO , GO_2 , $SO_7(G)$, $SO_8(G)$, $SO_9(G)$, and $SO_{10}(G)$ are given for trees from 6 vertices up to 13 vertices.

Investigating the SS and Abr values of a topological index on a class of molecules means investigating the sensitivity of the topological index on similar molecules within a class of molecules. To explain briefly, the most desirable situation for a topological index in this research is to have as high an SS value as possible and as small an Abr value as possible, i.e. to have an Abr value as close to the SS value as possible, details can be found in [2, 10, 11]. Since we focus on the structures that are trees with 6 to 13 vertices, we first need to identify similar graphs in these graph classes. For this purpose, graphs with graph edit distance of 1 are taken as a basis, see [2] for details on graph edit distance.

Table 2 shows that SO_8 and SO_{10} have the highest SS and $\frac{SS}{Abr}$ values among the proposed indices. It is also noticeable that the sensitivity of SO_{10} is better than SO_8 as the number of vertices of the trees increases. In addition, as the number of vertices increases, it is observed that the sensitivity of SO_8 and SO_{10} are very close to the sensitivity of the related indices GO_2 and ESO , respectively.

In Table 3, the degeneracy values of ESO , GO_2 , $SO_7(G)$, $SO_8(G)$, $SO_9(G)$, and $SO_{10}(G)$ are shown for trees from 6 vertices to 13 vertices.

To the extent that a topological index encodes the structural properties of a molecule by using its graph model, it can be considered successful as a molecular descriptor. Whenever possible, a topological index with a low degeneracy value encodes more structural properties, for details we refer to [1, 7].

In Table 3, the indices SO_9 and SO_{10} have the more desirable degeneracy values (closest to zero) among the proposed indices as the number of vertices increases. At this point, SO_7 and SO_8 have worse performance due to higher degeneracy values than the others.

Table 2. *SS* and *Abr* values of the indices for trees from 6 vertices up to 13 vertices.

		6	7	8	9	10	11	12	13
<i>ESO</i>	SS	0,32035	0,27001	0,22721	0,19869	0,17389	0,15630	0,14096	0,12889
	Abr	0,50895	0,48184	0,45597	0,43696	0,41925	0,40641	0,39302	0,38008
	Proportion (SS/Abr)	0,62942	0,56038	0,49829	0,45472	0,41477	0,38459	0,35866	0,33910
<i>GO₂</i>	SS	0,28628	0,26213	0,24032	0,21963	0,20192	0,18703	0,17332	0,16184
	Abr	0,42371	0,47129	0,50982	0,53284	0,54550	0,55273	0,55386	0,55125
	Proportion (SS/Abr)	0,67567	0,55620	0,47138	0,41220	0,37015	0,33838	0,31293	0,29359
<i>SO₇</i>	SS	0,17036	0,16447	0,18103	0,17066	0,16920	0,16028	0,15287	0,14489
	Abr	0,30431	0,32504	0,39794	0,44647	0,48458	0,50709	0,51961	0,52357
	Proportion (SS/Abr)	0,55983	0,50601	0,45490	0,38223	0,34917	0,31608	0,29420	0,27673
<i>SO₈</i>	SS	0,40281	0,34822	0,29816	0,26554	0,23715	0,21625	0,19782	0,18295
	Abr	0,60197	0,60480	0,61336	0,62093	0,61855	0,61468	0,60824	0,59961
	Proportion (SS/Abr)	0,66915	0,57577	0,48611	0,42765	0,38339	0,35181	0,32524	0,30511
<i>SO₉</i>	SS	0,08349	0,08429	0,09441	0,08894	0,08753	0,08249	0,07835	0,07409
	Abr	0,14004	0,15793	0,19645	0,21500	0,23165	0,23822	0,24240	0,24199
	Proportion (SS/Abr)	0,59620	0,53373	0,48057	0,41368	0,37787	0,34627	0,32322	0,30617
<i>SO₁₀</i>	SS	0,44125	0,36339	0,29590	0,25638	0,22149	0,19726	0,17668	0,16061
	Abr	0,70794	0,65020	0,59917	0,56269	0,53052	0,50627	0,48374	0,46315
	Proportion (SS/Abr)	0,62329	0,55888	0,49384	0,45563	0,41750	0,38963	0,36524	0,34677

Moreover, it is observed that *SO₈* and *SO₁₀* have slightly lower degeneracy values (encode slightly more structural features) than the related *GO₂* and *ESO* indices, respectively.

Table 3. Degeneracy values of the indices for trees from 6 vertices to 13 vertices.

	<i>ESO</i>	<i>GO₂</i>	<i>SO₇</i>	<i>SO₈</i>	<i>SO₉</i>	<i>SO₁₀</i>
6 vertices	0,00000	0,00000	0,16667	0,00000	0,00000	0,00000
7 vertices	0,00000	0,09091	0,36364	0,00000	0,00000	0,00000
8 vertices	0,08696	0,13043	0,34783	0,08696	0,04348	0,08696
9 vertices	0,14894	0,25532	0,51064	0,17021	0,12766	0,12766
10 vertices	0,24528	0,39623	0,62264	0,29245	0,20755	0,18868
11 vertices	0,33617	0,53617	0,73617	0,46383	0,29787	0,28936
12 vertices	0,41924	0,68966	0,82033	0,61162	0,38475	0,40109
13 vertices	0,50576	0,79862	0,90161	0,74712	0,45888	0,49116

Table 4. Mutual $|R|$ values of the indices for decane isomers.

	<i>ESO</i>	<i>GO₂</i>	<i>SO₈</i>	<i>SO₁₀</i>
<i>ESO</i>	1	0,93761	0,99058	0,97716
<i>GO₂</i>		1	0,88693	0,97441
<i>SO₈</i>			1	0,95608
<i>SO₁₀</i>				1

Table 4 shows the mutual correlations of *SO₈*, *SO₁₀*, *GO₂* and *ESO* indices. From this table, $|R| < 0.89$ for the correlation between *SO₈* and *GO₂* while $|R| > 0.97$ for the

correlation between SO_{10} and ESO . That is, SO_8 and GO_2 are not very similar in chemical applicability potential, whereas SO_{10} has a high chemical applicability potential similarity with ESO .

As a result of the research carried out in this section, it can be concluded that although SO_8 and SO_{10} do not have a high chemical applicability potential but have a better chemical applicability potential among the other proposed indices.

4 Extremal trees and connected graphs for the y -line volume index and y -surface area index

In this section, we focus on SO_8 and SO_{10} as they outperform the others in terms of chemical applicability potential. Connected graphs and trees that attain the extremal values for SO_8 and SO_{10} are determined among all connected graphs and trees, respectively.

Theorem 4.1. *Let $G = (V, E)$ be a connected graph with $n \geq 3$ vertices and m edges. Let $d_u \geq d_v$. Then,*

$$8n - 16 \leq SO_8(G) \leq \frac{1}{2}n(n-1)^4.$$

The left and right equalities hold if and only if $G \cong P_n$ and $G \cong K_n$, respectively.

Proof. Let $G = (V, E)$ be a connected graph with $n \geq 3$ vertices, and $d_u \geq d_v$. Since it is clear that deleting an edge from graph G necessarily reduces $SO_8(G)$, the connected graph with minimum $SO_8(G)$ must be a tree.

Let us denote $m(d_v, d_u)$ and $r(d_v, d_u)$ as the number of edges connecting vertices of degree d_v and d_u in graph G and the contribution of edge uv to the corresponding topological index, respectively.

Since

$$r(1, 2) = 4 < r(2, 2) = 8 < r(1, 3) = 9 < \dots$$

for $SO_8(G)$, then we obtain that

$$\sum_{uv \in E} d_u^2 \cdot d_v \geq m(1, 2)r(1, 2) + m(2, 2)r(2, 2).$$

Equality holds if and only if $G \cong P_n$. Therefore, since equality is realized in the case of P_n and $m(1, 2) = 2, m(2, 2) = n - 3$ for P_n , we get the lower bound as $2 \cdot 2^2 \cdot 1 + (n - 3) \cdot 2^2 \cdot 2 = 8n - 16$.

Since K_n is the only simple connected graph with $m = \frac{1}{2}n(n-1)$, where all vertices have degree $n-1$, which is the maximum possible degree of a vertex in a simple connected graph, the upper bound of $SO_8(G)$ is obtained as $SO_8(K_n) = \frac{1}{2}n(n-1)^4$. $\square$

Theorem 4.2. *Let $G = (V, E)$ be a connected graph with $n \geq 3$ vertices, and $d_u \geq d_v$. Then,*

$$4\sqrt{5} + 2(n-3)\sqrt{8} \leq SO_{10}(G) \leq \frac{1}{\sqrt{2}}n(n-1)^3.$$

The left and right equalities hold if and only if $G \cong P_n$ and $G \cong K_n$, respectively.

Proof. Let $G = (V, E)$ be a connected graph with $n \geq 3$ vertices, and $d_u \geq d_v$. Starting from the expression presented for SO_8 in the proof of Thm. 4.1, the connected graph with minimum $SO_{10}(G)$ must be a tree.

Assume that the notations $m(d_v, d_u)$ and $r(d_v, d_u)$ are used as given in the proof of Thm. 4.1.

Since $r(d_v, d_u) = d_u \sqrt{d_u^2 + d_v^2}$, it is easy to observe that

$$r(1, 2) = 2\sqrt{5} < r(2, 2) = 2\sqrt{8} < r(1, 3) = 3\sqrt{10} < \dots$$

for $SO_{10}(G)$. Then the proof is completed as follows:

$$\sum_{uv \in E} d_u \sqrt{d_u^2 + d_v^2} \geq m(1, 2)r(1, 2) + m(2, 2)r(2, 2).$$

It is clear that equality holds if and only if $G \cong P_n$. Therefore, since $m(1, 2) = 2$ and $m(2, 2) = n - 3$ for P_n , we get that

$$\sum_{uv \in E} d_u \sqrt{d_u^2 + d_v^2} \geq 4\sqrt{5} + 2(n - 3)\sqrt{8}.$$

Equality holds if and only if $G \cong P_n$.

By following the same explanation that is explained in the proof of Thm. 4.1 for K_n , the upper bound of $SO_{10}(G)$ is obtained as $SO_{10}(K_n) = \frac{1}{\sqrt{2}}n(n - 1)^3$. $\square$

Theorem 4.3. Let $T = (V, E)$ be a tree with $n \geq 3$ vertices, and $d_u \geq d_v$. Then,

$$8n - 16 \leq SO_8(T) \leq (n - 1)^3.$$

The left and right equalities hold if and only if $T \cong P_n$ and $T \cong S_n$, respectively.

Proof. The lower bound follows from Thm 4.1.

Let us focus on the upper bound. Let $T = (V, E)$ be a tree with $n \geq 3$ vertices. It is obvious that $SO_8(T) \leq (n - 1)^3$ is satisfied for $n = 3, 4, 5$ and equality holds if and only if $T \cong S_n$. One can deduce that $d_u + d_v \leq n$ for all edges of T . Moreover, the following inequality holds for $SO_8(T)$, where $n \geq 6$:

$$\dots < r(3, n - 3) = 3(n - 3)^2 < r(2, n - 2) = 2(n - 2)^2 < r(1, n - 1) = (n - 1)^3.$$

As a result, it is achieved that

$$\sum_{uv \in E} d_u^2 \cdot d_v \leq (n - 1)r(1, n - 1) = (n - 1)^3.$$

Equality holds if and only if $T \cong S_n$. $\square$

Theorem 4.4. Let $T = (V, E)$ be a tree with $n \geq 3$ vertices, and $d_u \geq d_v$. Then,

$$4\sqrt{5} + 2(n - 3)\sqrt{8} \leq SO_{10}(T) \leq (n - 1)^2 \sqrt{n^2 - 2n + 2}.$$

The left and right equalities hold if and only if $T \cong P_n$ and $T \cong S_n$, respectively.

Proof. The lower bound follows from Thm. 4.2.

Let $T = (V, E)$ be a tree with $n \geq 3$ vertices. It is easy to observe that $SO_{10}(T) \leq (n-1)^2 \sqrt{n^2 - 2n + 2}$ is satisfied for $n = 3, 4, 5$ and equality holds if and only if $T \cong S_n$. As mentioned in the proof of Thm. 4.3, it is known that $d_u + d_v \leq n$ for all edges of T . Furthermore, it can be observed that the following inequality holds for $SO_{10}(T)$, where $n \geq 6$:

$$\dots < r(3, n-3) < r(2, n-2) < r(1, n-1) = (n-1) \cdot \sqrt{(n-1)^2 + 1^2}.$$

Then, it is obtained that

$$\begin{aligned} \sum_{uv \in E} d_u \sqrt{d_u^2 + d_v^2} &\leq (n-1) \cdot r(1, n-1) \\ &\leq (n-1)^2 \sqrt{n^2 - 2n + 2}. \end{aligned}$$

Equality holds if and only if $T \cong S_n$. □

Let us now present the relations between SO_8 and SO_{10} with the SO , respectively.

Theorem 4.5. *Let $G = (V, E)$ be a connected graph with n vertices, and $d_u \geq d_v$. Then*

$$\frac{1}{2}SO(G) < SO_8(G) \leq \frac{(n-1)^2}{\sqrt{2}}SO(G).$$

Equality holds if and only if $G \cong K_n$.

Proof. Let $G = (V, E)$ be a connected graph with n vertices, and $d_u \geq d_v$. By using some simple mathematical properties together with $d_u \geq d_v$ it can be observed that

$$d_u^2 \geq d_u > \frac{1}{2}\sqrt{2d_u^2} \geq \frac{1}{2}\sqrt{d_u^2 + d_v^2}.$$

By using equality above, we get the following inequality:

$$\begin{aligned} SO_8(G) &= \sum_{uv \in E} d_u^2 \cdot d_v \\ &\geq \sum_{uv \in E} d_u^2 \\ &> \sum_{uv \in E} \frac{1}{2}\sqrt{d_u^2 + d_v^2} \\ &= \frac{1}{2}SO(G). \end{aligned}$$

Since $(d_u - d_v)^2 \geq 0$ with equality $d_u = d_v$, it is achieved that $\frac{d_u^2 + d_v^2}{2} \geq d_u d_v$ with equality $d_u = d_v$. By following this inequality, it is obtained that

$$\begin{aligned}
 SO_8(G) &= \sum_{uv \in E} d_u^2 \cdot d_v \\
 &\leq \sum_{uv \in E} d_u \left(\frac{d_u^2 + d_v^2}{2} \right), \text{ with equality } d_u = d_v \\
 &= \sum_{uv \in E} d_u \sqrt{d_u^2 + d_v^2} \left(\frac{\sqrt{d_u^2 + d_v^2}}{2} \right) \\
 &\leq \sum_{uv \in E} \frac{1}{2} (n-1) \sqrt{2(n-1)^2} \sqrt{d_u^2 + d_v^2}, d_u = d_v = n-1 \text{ for all edges} \\
 &= \frac{(n-1)^2}{\sqrt{2}} SO(G).
 \end{aligned}$$

It is obvious that equality holds if and only if $G \cong K_n$. □

Theorem 4.6. Let $G = (V, E)$ be a connected graph with n vertices, and $d_u \geq d_v$. Then

$$SO(G) \leq SO_{10}(G) \leq (n-1) SO(G).$$

The left equality holds if and only if $G \cong P_2$.

Proof. Let $G = (V, E)$ be a connected graph with n vertices, and $d_u \geq d_v$. Since $d_u = 1$ and $d_u = n-1$ are the minimum and maximum possible degrees of vertices in G , respectively, it is clear that

$$SO(G) = \sum_{uv \in E} \sqrt{d_u^2 + d_v^2} \leq \sum_{uv \in E} d_u \sqrt{d_u^2 + d_v^2} \leq \sum_{uv \in E} (n-1) \sqrt{d_u^2 + d_v^2} = (n-1) SO(G).$$

The left equality holds if and only if $G \cong P_2$. □

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