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Research Article

More geometric studies of vertex-degree-based graph indices–tangent Sombor index

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Abstract

The representation of an edge of a graph in a 2-dimensional coordinate system (shown in Fig. 1) made it possible to get a geometric interpretation of several earlier proposed vertex-degree-based graph indices. In particular, the sum of sine, cosine, and secant of the angle α (shown in Fig. 1) over all edges of the underlying graph yields, respectively, the second Sombor, inverse symmetric division deg, and symmetric division deg indices. Analogous trigonometric relations for the cosecant and cotangent of α are not possible. Therefore, the only remaining such relation is for the tangent of α, resulting in a new vertex-degree-based topological index, the *tangent Sombor index*, Tan.
In this paper, the basic properties of Tan are established. Connected graphs and trees reaching extremal Tan-values are characterized. Inequalities between Tan and other graph indices are established. The chemical usefulness of Tan in terms of structure sensitivity, abruptness, degeneracy, and correlation with some physicochemical properties of octane isomers and other indices is investigated.

Mathematics Subject Classification (2020). 05C09, 05C90, 05C92

Keywords. tangent Sombor index, Sombor index, topological index

1. Introduction

Let $G = (V, E)$ be a simple graph with vertex set V and edge set E. The degree of a vertex $u \in V$ is denoted by d_u. An edge $e \in E$ connecting the vertices $u, v \in V$ is denoted by $e = uv$.

Nowadays, in the mathematical and chemical literature, there exist several dozens of vertex-degree-based (VDB) graph indices (usually referred to as "topological indices"), some of which have found important chemical or pharmacological applications. These indices are intensively investigated from both chemical and mathematical points of view [10, 17, 28]. Their general mathematical form is:

$$TI(G) = \sum_{uv \in E} F(d_u, d_v)\,, \tag{1.1}$$

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where $F(x,y)$ is some function with the property $F(x,y) = F(y,x)$, defined for all values of x, y that the vertex degrees of a graph may assume.

Some of the VDB graph indices that we are considering within the present study are: the second Zagreb index [14]

$$M_2(G) = \sum_{uv \in E} d_u \, d_v \,,$$

the Albertson index [1]

$$Alb\,(G) = \sum_{uv \in E} |d_u - d_v| \,,$$

the general Randić index for $\alpha = -1$ [4]

$$R_{-1}\,(G) = \sum_{uv \in E} \frac{1}{d_u \, d_v} \,,$$

the symmetric division deg index [2, 29]

$$SDD(G) = \sum_{uv \in E} \left(\frac{d_u}{d_v} + \frac{d_v}{d_u} \right) \,, \tag{1.2}$$

the inverse symmetric division deg index [9]

$$ISDD(G) = \sum_{uv \in E} \frac{d_u \, d_v}{d_u^2 + d_v^2} \,, \tag{1.3}$$

and the Sombor index [11]

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

In a recent paper [11], it was noticed that the vertex pair (d_u, d_v) in formula (1.1) can be given a geometric interpretation, as shown in Fig. 1.

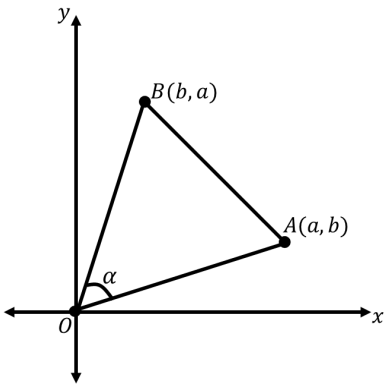

Figure 1. A geometric representation of an edge $e = uv$ of a graph G, connecting vertices of degree $d_u = a$ and $d_v = b$ $(a > b)$. Point A corresponds to the ordered pair (d_u, d_v), whereas its dual, denoted by B, to the pair (d_v, d_u). The (Euclidean) distance between A and the origin O (or the equal distance between B and O), summed over all edges, was used for the definition of the Sombor index. The distance between A and B pertains to the Albertson index. The angle between the lines AO and BO is denoted by $\alpha = \alpha_{uv}$.

The Sombor index is the first VDB graph index designed by means of geometry-based consideration (cf. Fig. 1). Eventually, it found remarkable chemical [18, 22, 23] and other [3, 24] applications, and its mathematical properties were studied in due detail,

see the review [19]. Motivated by its success, further geometry-based studies have been undertaken, resulting in design of several new VDB graph indices [8, 12, 13, 15, 27].

In [12], the following six Sombor-index-like VDB graph indices were put forward, all related to the triangle ABO in Fig. 1.

$$SO_1(G) = \frac{1}{2}\sum_{uv\in E}\left|d_u^2 - d_v^2\right|, \qquad SO_2(G) = \sum_{uv\in E}\frac{|d_u^2 - d_v^2|}{d_u^2 + d_v^2},$$

$$SO_3(G) = \sqrt{2}\pi\sum_{uv\in E}\frac{d_u^2 + d_v^2}{d_u + d_v} \qquad SO_4(G) = \frac{\pi}{2}\sum_{uv\in E}\left(\frac{d_u^2 + d_v^2}{d_u + d_v}\right)^2,$$

$$SO_5(G) = 2\pi\sum_{uv\in E}\frac{|d_u^2 - d_v^2|}{\sqrt{2} + 2\sqrt{d_u^2 + d_v^2}}, \qquad SO_6(G) = \pi\sum_{uv\in E}\left(\frac{d_u^2 - d_v^2}{\sqrt{2} + 2\sqrt{d_u^2 + d_v^2}}\right)^2.$$

Of these, SO_2 is related to the angle $\alpha = \alpha_{uv}$, whose geometric meaning is explained in Fig. 1. In particular,

$$SO_2(G) = \sum_{uv\in E}\sin\alpha_{uv} \tag{1.4}$$

where, as shown in [12],

$$\sin\alpha = \frac{|d_u^2 - d_v^2|}{d_u^2 + d_v^2}\,. \tag{1.5}$$

In [25], the topological index SO_2 was named "*second Sombor index*" and was eventually studied in much detail [8, 25, 26].

Knowing $\sin\alpha$, Eq. (1.5), the analogous expressions for other trigonometric functions of α are straightforwardly obtained:

$$\cos\alpha = \sqrt{1 - \sin^2\alpha} = \frac{2d_u\,d_v}{d_u^2 + d_v^2} \tag{1.6}$$

$$\sec\alpha = \frac{1}{\cos\alpha} = \frac{d_u^2 + d_v^2}{2d_u\,d_v} \tag{1.7}$$

$$\csc\alpha = \frac{1}{\sin\alpha} = \frac{d_u^2 + d_v^2}{|d_u^2 - d_v^2|} \tag{1.8}$$

$$\tan\alpha = \frac{\sin\alpha}{\cos\alpha} = \frac{|d_u^2 - d_v^2|}{2d_u\,d_v} \tag{1.9}$$

$$\cot\alpha = \frac{\cos\alpha}{\sin\alpha} = \frac{2d_u\,d_v}{|d_u^2 - d_v^2|}\,. \tag{1.10}$$

Observation 1.1. Bearing in mind that

$$\frac{d_u^2 + d_v^2}{d_u\,d_v} = \frac{d_u}{d_v} + \frac{d_v}{d_u}$$

we see that the symmetric division deg index SDD, Eq. (1.2), is related to the secant of α as

$$SDD(G) = 2\sum_{uv\in E}\sec\alpha_{uv}\,.$$

Observation 1.2. Analogously, the inverse symmetric division deg index $ISDD$, Eq. (1.3), is related to the cosine of α as

$$ISDD(G) = \frac{1}{2} \sum_{uv \in E} \cos \alpha_{uv} \, .$$

Observation 1.3. The cosecant and cotangent of α cannot be related to any VDB index because there are graphs possessing edges uv for which $d_u = d_v$ and then the divisor on the right-hand sides of Eqs. (1.8) and (1.10) is zero.

Bearing in mind Eq. (1.4) and Observations 1.1–1.3, we see that the only remaining trigonometric function of α is the tangent. This motivates us to consider a new VDB graph index defined as

$$Tan = Tan(G) = \sum_{uv \in E} \tan \alpha_{uv}$$

or, by Eq. (1.9),

$$Tan = Tan(G) = \sum_{uv \in E} \frac{|d_u^2 - d_v^2|}{2 d_u \, d_v} \, .$$

We prefer to call Tan the *tangent Sombor index*.

In what follows, we characterize extremal graphs and trees in the class of all graphs and trees. Moreover, we provide bounds for Tan in terms of some other well-known VDB indices. In the last section, we investigate the chemical applicability potential of this index in the context of structure sensitivity, abruptness, degeneracy, and its correlation with various thermodynamic properties.

2. Basic mathematical properties of tangent Sombor index

Let us denote $w_{d_j,d_i} = \dfrac{\left|d_i^2 - d_j^2\right|}{2 d_i \, d_j}$ as the contribution to $Tan(G)$ of the edge ij. Note that P_n, S_n, K_n represent the path graph, star graph and complete graph of order n, respectively.

Theorem 2.1. *Let $G = (V, E)$ be a connected graph with $n \geq 2$ vertices and m edges. Then,*

$$0 \leq Tan\,(G) \leq m \frac{\Delta^2 - \delta^2}{2 \Delta \delta},$$

where Δ and δ are the maximum and minimum vertex degrees among all vertices in G, respectively. The left and right equalities hold if and only if G is a regular graph and G is the graph where $max\,\{d_i, d_j\} = \Delta$ and $min\,\{d_i, d_j\} = \delta$ for each edge, respectively.

Proof. It is evident that $Tan\,(G)$ reaches the minimum value when $d_i^2 - d_j^2 = 0$ for all edges. Since this is satisfied in the case of G is a regular graph, the lower bound is proved.

Focusing on the upper bound, without loss of generality let us assume that $d_i \geq d_j$. For any connected graph G with $n \geq 2$ vertices, the following inequality holds:

$$\frac{\delta}{\Delta} \leq \frac{d_j}{d_i} \leq 1.$$

Let us define a function in such a way that

$$f\left(\frac{d_j}{d_i}\right) = \frac{d_i^2 - d_j^2}{2 d_i \, d_j} = \frac{1 - \left(\dfrac{d_j}{d_i}\right)^2}{2 \dfrac{d_j}{d_i}}.$$

It is clear that the function $f(x) = \dfrac{1-x^2}{2x}$ is a decreasing function on the interval $\left(\dfrac{\delta}{\Delta}, 1\right)$ using the first derivative $f'(x) = \dfrac{-2x^2-2}{4x^2}$.

Then the maximum value of the function $f\left(\dfrac{d_j}{d_i}\right)$ on the interval $\left(\dfrac{\delta}{\Delta}, 1\right)$ is obtained when $d_j = \delta, d_i = \Delta$. As a result, $Tan(G)$ reaches the maximum value for graphs with $max\{d_i, d_j\} = \Delta$ and $min\{d_i, d_j\} = \delta$ for each edge $ij \in E$ and the maximum value is $Tan(G) = m\dfrac{\Delta^2 - \delta^2}{2\Delta\delta}$. □

Theorem 2.2. *Let $T = (V, E)$ be a tree with $n \geq 2$ vertices. Then,*

$$Tan(P_n) \leq Tan(T) \leq Tan(S_n).$$

The left and right equalities hold if and only if $T \cong P_n$ and $T \cong S_n$, respectively. Moreover $Tan(P_2) = 0$ and $Tan(P_n) = \dfrac{3}{2}$ when $n \geq 3$. Furthermore, $Tan(S_n) = \dfrac{(n-1)(n^2-2n)}{2n-2}$ when $n \geq 2$.

Proof. In the proof of Theorem 2.1, it is stated that when $d_i^2 - d_j^2 = 0$ for all edges, $Tan(T)$ reaches the minimum value. However, when working with trees, there is no tree except P_2 satisfying the condition $d_i = d_j$ for all edges. It is already known that $Tan(P_2) = 0$. For $n \geq 3$, trees by nature must contain at least 2 pendant edges. At this point, let us consider $w_{1,d_i} = \dfrac{d_i^2 - 1}{2d_i}$. By considering the function $f(x) = \dfrac{x^2-1}{2x}$ with the domain $2 \leq x \in \mathbb{N}$ and $f'(x) = \dfrac{2x^2+2}{4x^2} > 0$, it can be deduced that f is increasing. As a result, it is obtained that

$$w_{1,2} < w_{1,3} < \cdots < w_{1,n-1}.$$

Hence, for P_n, which has just 2 pendant vertices and the other edges are the edges connecting the vertices of degree 2, it achieves the minimum value, which is $Tan(P_n) = 2w_{1,2} = 2\dfrac{3}{4} = \dfrac{3}{2}$.

As for the upper bound, since the number of edges in a tree T with n vertices is $n-1$, the maximum possible vertex degree in T is $n-1$, and the minimum possible vertex degree in T is 1, the result is obtained using Thm. 2.1 as follows:

$$Tan(T) \leq Tan(S_n) = (n-1)\frac{(n-1)^2 - 1^2}{2 \cdot 1 \cdot (n-1)} = \frac{(n-1)(n^2-2n)}{2n-2}$$

□

Let us recall Radon's inequality for future use.

Lemma 2.3. [20] *Let $x_1, x_2, \ldots, x_k, r$ be nonnegative real numbers and $y_1, y_2, \ldots, y_k$ be positive real numbers. Then the following inequality holds:*

$$\sum_{i=1}^{k} \frac{x_i^{r+1}}{y_i^r} \geq \frac{\left[\sum_{i=1}^{k} x_i\right]^{r+1}}{\left[\sum_{i=1}^{k} y_i\right]^r}.$$

Equality holds if and only if $\dfrac{x_1}{y_1} = \dfrac{x_2}{y_2} = \cdots = \dfrac{x_k}{y_k}$.

Theorem 2.4. *Let $G = (V, E)$ be a connected graph with $n \geq 2$ vertices and m edges. Then,*

$$\frac{Alb(G)}{2M_2(G)} \leq Tan(G) \leq \frac{1}{2}SDD(G) + R_{-1}(G).$$

The left and right equalities hold if and only if G is a regular graph and $G \cong S_n$, respectively.

Proof. First, let us focus on the lower bound. It is clear that $\left|d_i^2 - d_j^2\right| \geq |d_i - d_j|$, where $d_i, d_j \in \mathbb{N}^+$. Equality holds if and only if $d_i = d_j$. Hence, we get the following inequality:

$$Tan\,(G) = \sum_{ij\in E} \frac{\left|d_i^2 - d_j^2\right|}{2d_i\,d_j} \geq \sum_{ij\in E} \frac{|d_i - d_j|}{2d_i\,d_j} = \sum_{ij\in E} \frac{\sqrt{|d_i - d_j|}^2}{2d_i\,d_j},$$

with the equality in the case of $d_i = d_j$ for all edges of G. Then, using Radon's inequality leads to the following inequality:

$$Tan(G) \geq \sum_{ij\in E} \frac{\sqrt{|d_i - d_j|}^2}{2d_i\,d_j} \geq \frac{\left(\sum_{ij\in E}\sqrt{|d_i - d_j|}\right)^2}{2\sum_{ij\in E} d_i\,d_j}$$

with the equality if and only if G is a regular graph. Furthermore, it is obtained the following inequality by using some simple mathematical properties:

$$\begin{aligned} Tan(G) &\geq \frac{\left(\sum_{ij\in E}\sqrt{|d_i - d_j|}\right)^2}{2\sum_{ij\in E} d_i\,d_j}, \\ &\geq \frac{\sqrt{\sum_{ij\in E}|d_i - d_j|}^2}{2\sum_{ij\in E} d_i\,d_j} \text{ with the equality in the case of } d_i = d_j \text{ for all edges of } G, \\ &= \frac{\sum_{ij\in E}|d_i - d_j|}{2\sum_{ij\in E} d_i\,d_j} = \frac{Alb(G)}{2M_2(G)}. \end{aligned}$$

Equality holds if and only if G is a regular graph.

Let us investigate the upper bound. The triangle inequality shows that

$$\left|x_1^2 - x_2^2\right| < x_1^2 + x_2^2, \tag{2.1}$$

where $x_1, x_2 \in \mathbb{N}^+$.
Thus, by using Eq. (2.1), it is clear that $x_1^2 + x_2^2 - |x_1^2 - x_2^2|$ reaches the minimum value when $x_1 = x_2 = 1$ for $x_1, x_2 \in \mathbb{N}^+$. Therefore, for an edge of G, it can be seen that the inequality

$$\left|d_i^2 - d_j^2\right| \leq d_i^2 + d_j^2 - 2$$

exists by considering the smallest vertex degree pair $d_i = 1, d_j = 1$. Moreover, one can observe that the equality holds if and only if the low-degree end vertex of the edge is 1. Using this inequality, the following result is obtained:

$$\begin{aligned} Tan(G) &= \sum_{ij\in E} \frac{\left|d_i^2 - d_j^2\right|}{2d_i\,d_j} \leq \sum_{ij\in E} \frac{d_i^2 + d_j^2 - 2}{2d_i\,d_j} = \frac{1}{2}\left[\sum_{ij\in E} \frac{d_i^2 + d_j^2}{d_i\,d_j} - 2\sum_{ij\in E} \frac{1}{d_i\,d_j}\right] \\ &= \frac{1}{2}\left[\sum_{ij\in E}\left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right) - 2\sum_{ij\in E}(d_i\,d_j)^{-1}\right] = \frac{1}{2}SDD\,(G) - R_{-1}(G)\,. \end{aligned}$$

Since the degree of the low-degree end vertex of all edges of S_n is 1, the equality holds if and only if $G \cong S_n$. □

3. Chemical applicability potential of tangent Sombor index

The thermodynamic properties of octane isomers given in Table 1, acentric factor (AcenFac), standard enthalpy of vaporization (DHVAP), entropy, enthalpy of vaporization (Hvap) were obtained from [5], also boiling point, and enthalpy of formation were obtained from [30].

In Table 1, the absolute values of Pearson correlation coefficients ($|R|$) values between the indices and the indicated chemical properties of octane isomers are presented.

	$SO_1(G)$	$SO_2(G)$	$SO_3(G)$	$SO_4(G)$	$SO_5(G)$	$SO_6(G)$	$ISDD(G)$	$SDD(G)$	$SO(G)$	$Tan(G)$
AcenFac	0.91920	0.92019	0.94819	0.94667	0.93033	0.90293	0.92463	0.90103	0.95942	0.93307
DHvap	0.95220	0.95610	0.95101	0.93001	0.97268	0.93790	0.97683	0.95278	0.94696	0.98066
Entropy	0.89015	0.84327	0.94008	0.94241	0.88927	0.90482	0.91033	0.91007	0.94659	0.91103
Hvap	0.91752	0.91982	0.91122	0.88373	0.93938	0.90531	0.95253	0.92767	0.90317	0.95052
Boiling P.	0.78107	0.79030	0.76011	0.72502	0.80734	0.77339	0.82347	0.80842	0.74330	0.82498
Enthalpy	0.82559	0.75893	0.81551	0.79538	0.82835	0.84476	0.85371	0.86117	0.79730	0.84820

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

It can be observed from Table 1 that $Tan(G)$ is comparable to $ISDD(G)$ and they have the best performance and second best performance for standard enthalpy of vaporization (DHVAP), enthalpy of vaporization (Hvap) and boiling point among all indices that exist in Table 1. Moreover, there is no significant difference between the $|R|$ values of the best performing indices for acentric factor, entropy, and enthalpy of formation and the $|R|$ value of the $Tan(G)$ index.

The following equations present regression models with standard error of the estimates (SEE) for $Tan\,(G)$ index.

$$\text{AcenFac} = -0.01382 \cdot Tan\,(G) + 0.41847, \text{ where SEE is equal to } 0.01314.$$

$$\text{DHvap} = -0.15700 \cdot Tan\,(G) + 10.06614, \text{ where SEE is equal to } 0.07734.$$

$$\text{Entropy} = -1.71851 \cdot Tan\,(G) + 115.70164, \text{ where SEE is equal to } 1.91964.$$

$$\text{Hvap} = -0.80442 \cdot Tan\,(G) + 73.97868, \text{ where SEE is equal to } 0.64883.$$

$$\text{Boiling P.} = -2.11638 \cdot Tan\,(G) + 399.51332, \text{ where SEE is equal to } 3.57822.$$

$$\text{Enthalpy} = -1.86454 \cdot Tan\,(G) - 205.70533, \text{ where SEE is equal to } 2.87356.$$

In Table 2, degeneracy values of the indices are presented for octanes, nonanes, decanes, and trees with $6, 7, \ldots, 12$ and 13 vertices.

In this study, the method proposed by Konstantinova in [16] for evaluating the degeneracy of a topological index is used. A topological index with lower degeneracy capture more structural information, namely lower degeneracy provides higher discriminative power [6].

Accordingly, Table 2 shows that the index with the highest discriminative power among the indices analyzed is $SO_4\,(G)$, while the index with the lowest discriminative power is $SO_1(G)$.

The discriminative powers of other indices with a degeneracy value between the degeneracy values of $SO_4(G)$ and $SO_1(G)$ indices are quite similar to each other. When the discriminative powers of these indices are compared with the discriminative power of $Tan(G)$, it is seen that the maximum value of the degeneracy value difference is approximately 0.08. In addition, based on octane, nonane and decane isomers, $Tan(G)$ is able to distinguish approximately 88%, 80% and 66% of these isomers, respectively.

	$SO_1(G)$	$SO_2(G)$	$SO_3(G)$	$SO_4(G)$	$SO_5(G)$	$SO_6(G)$	$ISDD(G)$	$SDD(G)$	$SO(G)$	$Tan(G)$
Octanes	0.50000	0.11111	0.05556	0.05556	0.11111	0.11111	0.05556	0.11111	0.11111	0.11111
Nonanes	0.65714	0.20000	0.14286	0.11429	0.20000	0.17143	0.08571	0.20000	0.17143	0.20000
Decanes	0.78667	0.34667	0.28000	0.22667	0.32000	0.32000	0.29333	0.32000	0.30667	0.33333
6 vertices	0.16667	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
7 vertices	0.27273	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
8 vertices	0.43478	0.08696	0.04348	0.04348	0.08696	0.08696	0.04348	0.08696	0.08696	0.08696
9 vertices	0.57447	0.14894	0.10638	0.08511	0.14894	0.12766	0.06383	0.14894	0.12766	0.14894
10 vertices	0.70755	0.25472	0.20755	0.16981	0.23585	0.23585	0.21698	0.23585	0.22642	0.24528
11 vertices	0.80000	0.30213	0.29362	0.22128	0.31064	0.31064	0.30213	0.34043	0.29362	0.32766
12 vertices	0.87296	0.40290	0.39020	0.32668	0.42831	0.41924	0.39746	0.48094	0.40472	0.45917
13 vertices	0.92314	0.49500	0.49424	0.43274	0.51729	0.50346	0.49347	0.60415	0.48655	0.56879

Table 2. Degeneracy values of the indices for octanes, nonanes, decanes, and trees with $6, 7, \ldots, 13$ vertices.

In Table 3, structure sensitivity (SS) and abruptness (Abr) values (with ratios) of the indices are presented for trees with $6, 7, \ldots, 12$ and 13 vertices.

		6	**7**	**8**	**9**	**10**	**11**	**12**	**13**
$SO_1(G)$	**SS**	1.07494	0.81580	0.60135	0.48720	0.39877	0.33955	0.29656	0.26419
	Abr	1.61806	1.35036	1.15274	1.01002	0.91481	0.83478	0.77716	0.72689
	Ratio	0.66434	0.60413	0.52167	0.48237	0.43591	0.40675	0.38159	0.36346
$SO_2(G)$	**SS**	0.45051	0.35102	0.26478	0.21961	0.18463	0.15894	0.14028	0.12581
	Abr	0.64811	0.56479	0.50563	0.45710	0.42109	0.38677	0.35947	0.33603
	Ratio	0.69512	0.62150	0.52365	0.48045	0.43846	0.41093	0.39024	0.37441
$SO_3(G)$	**SS**	0.22925	0.18721	0.15324	0.13167	0.11307	0.10019	0.08918	0.08064
	Abr	0.35426	0.31938	0.29372	0.27301	0.25466	0.24076	0.22776	0.21596
	Ratio	0.64713	0.58618	0.52172	0.48229	0.44403	0.41614	0.39154	0.37342
$SO_4(G)$	**SS**	0.46294	0.38254	0.31402	0.27201	0.23479	0.20928	0.18726	0.17015
	Abr	0.76988	0.71982	0.66164	0.62406	0.58623	0.55943	0.53314	0.50958
	Ratio	0.60131	0.53144	0.47460	0.43588	0.40051	0.37409	0.35125	0.33390
$SO_5(G)$	**SS**	0.79054	0.60290	0.44708	0.36385	0.2992	0.25456	0.22216	0.19764
	Abr	1.13413	0.92966	0.79497	0.69629	0.62692	0.56830	0.52594	0.48933
	Ratio	0.69704	0.64851	0.56239	0.52256	0.47725	0.44793	0.42240	0.40390
$SO_6(G)$	**SS**	1.53487	1.11517	0.81476	0.65420	0.52996	0.44952	0.38929	0.34502
	Abr	2.57338	2.10770	1.72740	1.51864	1.35383	1.22608	1.13038	1.05156
	Ratio	0.59644	0.52909	0.47167	0.43078	0.39146	0.36663	0.34438	0.32810
$ISDD(G)$	**SS**	0.25286	0.19457	0.15045	0.12187	0.09969	0.08475	0.07305	0.06436
	Abr	0.33822	0.28416	0.25342	0.22369	0.19928	0.18106	0.16547	0.15239
	Ratio	0.74761	0.68472	0.59370	0.54481	0.50023	0.46806	0.44145	0.42230
$SDD(G)$	**SS**	0.23593	0.19127	0.15463	0.13190	0.11193	0.09824	0.08664	0.07773
	Abr	0.36520	0.32663	0.29946	0.27726	0.25581	0.23995	0.22518	0.21221
	Ratio	0.64603	0.58557	0.51636	0.47571	0.43757	0.40941	0.38476	0.36631
$SO(G)$	**SS**	0.18346	0.15089	0.12455	0.10734	0.09260	0.08228	0.07344	0.06656
	Abr	0.28034	0.25486	0.23615	0.22042	0.20711	0.19689	0.18727	0.17836
	Ratio	0.65441	0.59205	0.52743	0.48699	0.44711	0.41788	0.39216	0.37316
$Tan(G)$	**SS**	0.68751	0.52638	0.40056	0.33089	0.27440	0.23520	0.20515	0.18244
	Abr	1.02777	0.85421	0.73494	0.65519	0.58867	0.53842	0.49737	0.46236
	Ratio	0.66893	0.61621	0.54502	0.50503	0.46613	0.43682	0.41248	0.39459

Table 3. Both structure sensitivity (SS) and abruptness (Abr) values (with ratios (SS/Abr)) of the indices for trees with $6, 7, \ldots, 12$ and 13 vertices.

The gradual change of any topological index values calculated on similar molecules as a result of gradual changes in the structure of a molecule was called the smoothness of the topological index in [7]. A useful model for measuring the smoothness of a topological

index is presented for the first time in [7] and is frequently used in chemical applicability potential investigations. This model includes the calculation of the structure sensitivity (SS) and abrubtness (Abr) values of the corresponding topological index.

In this study, the SS and Abr calculation method introduced in [7] is followed. A topological index with a value of SS as large as possible and a value of Abr as small as possible has a significant sensitivity to insufficient structural changes, for details we refer to [7, 21, 23]. In addition, from the formulae for Abr and SS presented in the method introduced in [7], it follows that the smallest possible value of Abr is equal to SS. In this respect, it can be said that a topological index with an SS/Abr value as close as possible to 1 has better performance.

Accordingly, if it is focused on the SS/Abr ratios of the trees as the number of vertices increases in Table 3, it is observed that $ISDD(G)$ has the best performance among all indices in Table 3 followed by $SO_5(G)$ and $Tan(G)$.

In Table 4, the absolute values of the mutual Pearson correlation coefficients ($|R|$) between $Tan(G)$, $ISDD(G)$, $SO(G)$ and some indices included in the mathematical lower and upper bounds of $Tan(G)$ presented in Theorem 2.4 are presented by using decane isomers.

	$M_2(G)$	$Alb(G)$	$R_{-1}(G)$	$SDD(G)$	$ISDD(G)$	$SO(G)$	$Tan(G)$
$M_2(G)$	1	0,80512	0,61860	0,77272	0,80627	0,88741	0,81078
$Alb(G)$		1	0,88125	0,96100	0,97774	0,97241	0,98900
$R_{-1}(G)$			1	0,96341	0,94506	0,88862	0,92961
$SDD(G)$				1	0,98810	0,97547	0,98513
$ISDD(G)$					1	0,98093	0,99619
$SO(G)$						1	0,98291
$Tan(G)$							1

Table 4. The absolute values of the mutual Pearson correlation coefficients ($|R|$) between $Tan(G)$, $M_2(G)$, $Alb(G)$, $R_{-1}(G)$, $SDD(G)$, $ISDD$ and $SO(G)$.

Table 4 shows that $Tan(G)$ has a strong correlation with the $ISDD(G)$. This indicates that the two indices have a close chemical applicability potential, which is also evident in Table 1.

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