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Original Article

Sombor, Nirmala, Dharwad, and F-Sombor Indices – A Comparative Study

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Abstract *- Let G be a molecular graph, d(u) the degree (number of first neighbors) of its vertex u, and uv its edge connecting the vertices u and v. In the recent literature, four vertex-degree-based molecular structure descriptors have been put forward, named Nirmala, Sombor, Dharwad, and F-Sombor indices, equal to the sum of the terms* $\sqrt{d(u)^k + d(v)^k}$ *over all edges uv of G for k=1,2,3, and 4. In this work, we compare these four indices. We find that they are highly correlated, and their value for QSPR applications is nearly the same. Therefore, only one (any one) of these topological indices should be used. From an applicative point of view, there was no need to introduce and study them separately.*

Keywords *- Sombor index, Nirmala index, Dharwad index, F-Sombor index, QSPR studies.*

Mathematics Subject Classification *- 05C05, 05C07, 05C09.*

1. Introduction

In Chemical Graph Theory [12,3,4], the mathematical apparatus of graph theory is applied for modeling chemical phenomena, mainly the relations between molecular structure and the properties (physicochemical, technological, biochemical, pharmacological, toxicological, …) of the underlying chemical compounds. For this, so-called *molecular graphs* are used, in which the *vertices* represent atoms and the *edges* represent chemical bonds. A popular technique is associating with the molecular graph a so-called *topological index* or *molecular structure descriptor*, namely a number representing certain structural features of the respective molecule [5]. The applications of topological indices usually go via constructing *quantitative structure-property relations* (QSPR) or *quantitative structure-activity relations* (QSAR), where "property" pertains to physicochemical, whereas "activity" refers to pharmacological or medicinal properties [5,6,7]. A large number of topological indices have been considered in the literature; for details, see [8,9].

In 2021, a new type of topological indices was put forward [10] using geometry-based considerations. This molecular structure descriptor, named the *Sombor index*, is defined as

$$SO = SO(G) = \sum_{uv} \sqrt{d(u)^2 + d(v)^2}$$

where u and v stand for two adjacent vertices of the molecular graph G, and $d(u)$ and $d(v)$ are the degrees (= number of first neighbors) of the vertices u and v, respectively. The edge of G connecting the vertices u and v is denoted by uv. The summation goes over all edges of the graph G.

Soon after its invention, the Sombor index found remarkably numerous chemical applications [11-19]; see also the review [20].

Motivated by the success of the Sombor index, several of its modified versions were introduced, first the Nirmala index [21]

$$N = N(G) = \sum_{uv} \sqrt{d(u) + d(v)}$$

then the Dharwad index [22]

$$Dh = Dh(G) = \sum_{uv} \sqrt{d(u)^3 + d(v)^3}$$

and quite recently, the F-Sombor index [23]

$$FSO = FSO(G) = \sum_{uv} \sqrt{d(u)^4 + d(v)^4}$$

Because of the close algebraic similarity of the four topological indices *SO*, *N*, *Dh*, and *FSO*, we found it purposeful to compare their mutual correlation and their performance in predicting physicochemical properties, i.e., possible usage in QSPR studies. The results of these comparative studies are outlined in the subsequent section.

2. Numerical Work

Figure 1 is shown the correlations between the Sombor index (horizontal axes) and the Nirmala, Dharwad, and F-Sombor indices (vertical axes). As expected, the regression lines are slightly non-linear, but nevertheless, their correlation coefficients are near-to-unity, equal to 0.9952, 0.9941, and 0.9790, respectively. Analogous correlations exist for trees and chemical trees with a number of vertices other than 10.

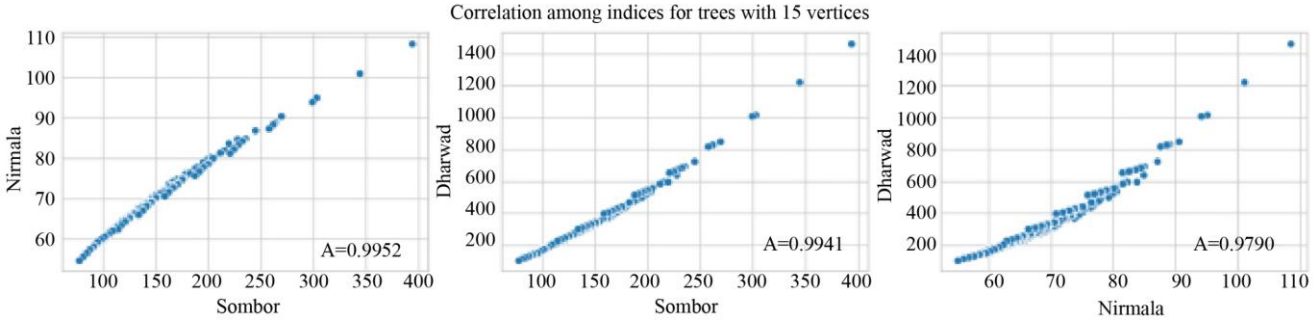

Fig. 1 The topological indices *N*, *Dh*, and *FSO* were plotted versus *SO* for 10-vertex trees

Since the topological indices *SO*, *N*, *Dh*, and *FSO* are mutually highly correlated, their predictive abilities w.r.t. physicochemical properties are expected to be similar. This, indeed, was found in the case of standard entropy (Figure 2), standard heats of vaporization (Figure 3), and acentric factors (Figure 4), where the correlations (and the respective correlation coefficients) differ insignificantly. Any topological indices *SO*, *N*, *Dh*, and *FSO*, could serve as a component of a QSPR model, but more than one would be superfluous.

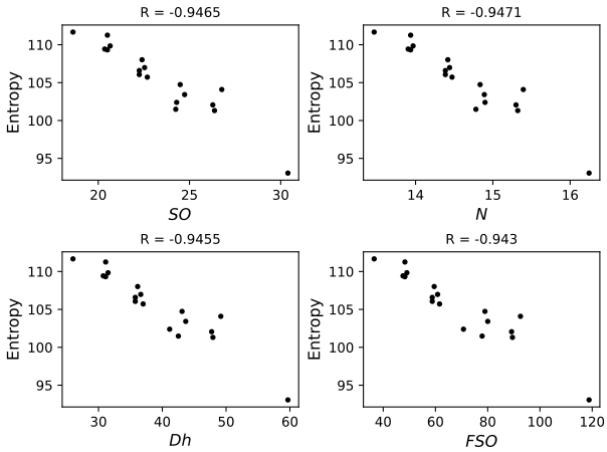

Fig. 2 Correlation of standard entropy of octane isomers with *SO, N, Dh, FSO*

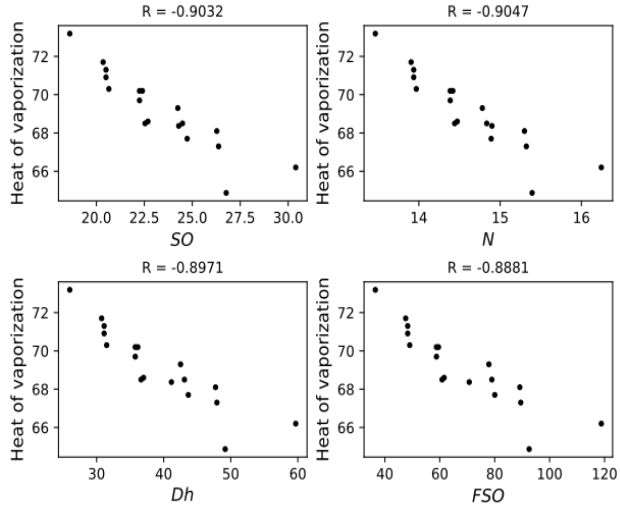

Fig. 3 Correlation of standard heats of vaporization of octane isomers with SO, N, Dh, FSO

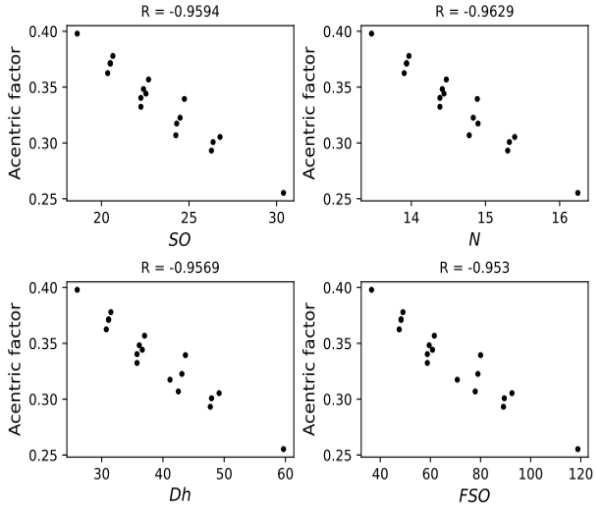

Fig. 4 Correlation of acentric factors of octane isomers with SO, N, Dh, FSO

We also present the respective plots for normal boiling points (Figure 5) and standard heats of formation (Figure 6), where any meaningful correlation is absent, equally for all four topological indices.

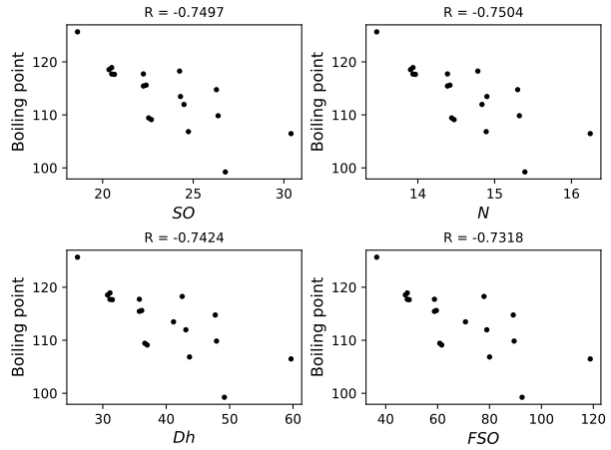

Fig. 5 Correlation of normal boiling points of octane isomers with SO, N, Dh, FSO

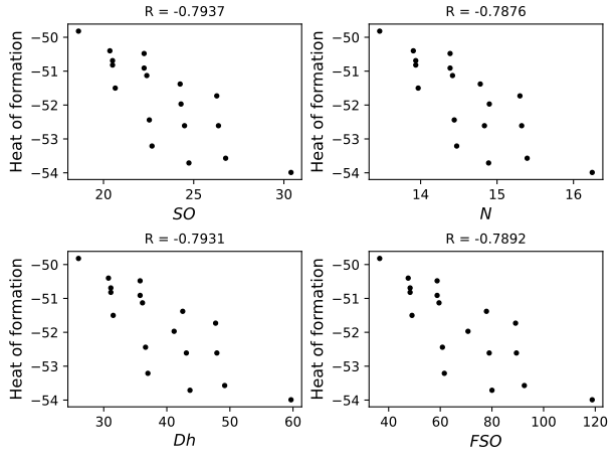

Fig. 6 Correlation of standard heats of formation of octane isomers with SO, N, Dh, FSO

3. Discussion and Concluding Remarks

The above-described numerical results hint towards the expectation that the basic mathematical properties of all vertex-degree-based graph invariant of the form

$$X = X(G) = \sum_{uv} \sqrt{d(u)^k + d(v)^k} \;\; ; \;\; k \geq 1$$

will be identical, independent of the actual value of the parameter *k*. That this indeed is the case is seen from the following results. Their proofs are analogous to those previously reported in [10, 22,24,25,26] and will therefore be skipped.

Theorem 1. Let *e* be any edge of the molecular graph *G*. Then $X(G-e) > X(G)$.

Corollary 1.1. Let *G* be any graph on *n* vertices, different from the edgeless graph E_n and the complete graph K_n. Then

$$0 = X(E_n) < X(G) < X(K_n) = \frac{n(n-1)}{2}\sqrt{2(n-1)^k}$$

Corollary 1.2. Among connected graphs with a fixed number of vertices, a tree has a minimal *X*-value.

Theorem 2. Let *G* be any graph. Then

$$\frac{1}{\sqrt{2}}\sum_u d(u)^{k/2+1} \leq X(G) < \sum_u d(u)^{k/2+1}$$

with summations going over all vertices. Equality on the left-hand side holds if and only if *G* is a regular graph (i.e., all vertices of *G* have mutually equal degrees).

Special cases of Theorem 2 for *k=2* and *k=4* are:

$$\frac{1}{\sqrt{2}} Zg(G) \leq SO(G) < Zg(G)$$

and

$$\frac{1}{\sqrt{2}} F(G) \leq FSO(G) < F(G)$$

Where *Zg* and *F* stand for the first Zagreb index [27] and the forgotten index [28], respectively.

Theorem 3. Let T_n be any tree on *n* vertices, different from the path P_n and the star S_n. Then

$$X(P_n) < X(T_n) < X(S_n)$$

i.e., among trees, the path has minimal and the star maximal *X*-value [26].

Theorem 4. Denote by C_n the *n*-vertex cycle and by W_n the graph obtained by attaching n-3 pendent vertices to a vertex of the triangle. Let U_n be any connected unicyclic graph on *n* vertices, different from the cycle C_n and W_n, then,

$$X(C_n) < X(U_n) < X(W_n)$$

i.e., among connected unicyclic graphs, the cycle has minimal and the graph W_n maximal *X*-value.

The main conclusion of the present work is that there is a great deal of redundancy between the Sombor, Nirmala, Dharwad, and F-Sombor topological indices. Therefore, only one (any one) among them should be used in QSPR and QSAR studies. From an applicative point of view, there was no need to introduce and study them separately. Since this already happened in the articles [10,21,22,23], two or more among these molecular structure descriptors should never be simultaneously employed.

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