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Research Article

Trinajstić index

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Abstract

Professor Trinajstić devoted years of research to deepen the knowledge of the distance–based topological indices. He was especially interested in so-called Szeged-type indices. Several such indices were introduced directly by himself, but none of them was named after him. In this paper, a novel topological invariant of this kind is proposed, and it is boldly named the *Trinajstić index*. The performed computational tests are justifying the introduction of this novel topological index.

Keywords: Trinajstić index; Szeged index; distance–based indices.

2020 Mathematics Subject Classification: 05C09, 05C92.

1. Introduction

Molecular descriptors give hope that the journey throughout endless chemical space won't be a random wandering but a methodical voyage toward substances of importance to mankind. Nowadays, there is a myriad of molecular descriptors, and among them, the topological indices have a prominent place.

The very first topological index was conceived in 1947 by Harry Wiener [18]. This index is known as the *Wiener index* and it is defined as the sum of distances between all pairs of vertices in a connected graph. However, in the seminal paper, the Wiener index of acyclic alkanes (trees) was calculated using Equation (1).

$$W(T) = \sum_{uv \in E(T)} n_u \cdot n_v \tag{1}$$

where n_u is the number of vertices that are closer to the vertex u (including the vertex u) than to vertex v.

This formula can be only used for calculating the Wiener index of trees. Researchers tried to extend the Equation (1) on graphs other than trees for almost 50 years. While there were some advances along this line of investigations, the complexity of obtained formulas was increasing. On the other hand, it was proposed in 1994 that the equality in (1) should be used for defining a novel index whose scope would not be limited only to trees. Thus, Equation (2) could be used in the entire realm of connected graphs. This new index was named *Szeged index* [5].

$$Sz(G) = \sum_{uv \in E(G)} n_u \cdot n_v \, . \tag{2}$$

Szeged index attracted a considerable attention in the researchers' cycles. Among other things, it was attractive to investigate the differences between the Szeged index and its ancestor, the Wiener index (see e.g. [1]). Such an intensive research has led to the emergence of many Szeged-like indices [2–4, 6, 7, 9, 12, 13, 16], and some of them were introduced by Trinajstić [3, 13] as well.

One of the first modifications on the definition of the Szeged index was done by Diudea et al. [2] who proposed the hyper–Szeged index. It is defined in the following way:

$$hSz(G) = \sum_{\{u,v\} \in V(G)} n_u \cdot n_v \tag{3}$$

where n_u and n_v are calculated in the same way as in the Equations (1) and (2). The summation goes over all unordered pairs of vertices in a connected graph G.

The other relative of the Szeged index that is important for a better understanding of the rest of the paper was introduced in 2002 by Randić [16]. Although, Randić named this index the *revised Wiener index*, nowadays it is better known as the

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revised Szeged index. In contrast to the original Szeged index, the equidistant vertices to the pair of end-vertices of an edge in a connected graph are also involved into definition of the revised Szeged index in the following manner:

$$rSz(G) = \sum_{uv \in E(G)} \left(n_u + \frac{n_0}{2}\right)\left(n_v + \frac{n_0}{2}\right). \tag{4}$$

The n_0 is the number of vertices equidistant to the end-vertices u and v.

Revised Szeged index was proposed to overcome the problem of underrated values of n-vertex non-bipartite connected graphs compared to their bipartite mates.

Trinajstić index

Combining the ideas that are incorporated in the indices' definitions (3) and (4), a novel topological index $\mathscr{X}(G)$ can be conceived as follows:

$$\mathscr{X}(G) = \sum_{\{u,v\} \in V(G)} \left(n_u + \frac{n_0}{2}\right)\left(n_v + \frac{n_0}{2}\right) \tag{5}$$

where n_u (respectively n_v) is the number of vertices of a connected graph G that are closer to vertex u (respectively v) than to vertex v (respectively u). The n_0 is the number of vertices that are equidistant to both vertices u and v. Summation goes over all unordered pairs of vertices in a connected graph G.

To the best knowledge of this author, the $\mathscr{X}(G)$ has never appeared earlier in the literature. Therefore, it could be a candidate for naming it after Prof. Trinajstić. However, I am inclined to propose a more elegant, and in the same time, a closely related index to be named after him. Namely, by the elementary algebraic simplifications, it can be easily shown that:

$$\mathscr{X}(G) = \frac{1}{8}n^3(n-1) - \frac{1}{4}\sum_{\{u,v\} \in V(G)} (n_u - n_v)^2. \tag{6}$$

Bearing in mind the fact that the majority of mathematical and chemical research on topological indices are focused on classes of connected graphs with a fixed order, the non-trivial part of the Equation (6) is interesting for further investigations. Therefore, I propose the *Trinajstić index* to be defined as follows:

$$\boxed{NT(G) = \sum_{\{u,v\} \in V(G)} (n_u - n_v)^2.} \tag{7}$$

From the definition of $NT(G)$ it is obvious that it can also be used as a measure of unbalancedness of a graph such as the total Mostar index [12].

A couple of elementary observations on the Trinajstić index will be outlined in the next few lines.

Observation 1.1. *If S_n is the star graph with n vertices, the Trinajstić index is equal to*

$$NT(S_n) = (n-1)(n-2)^2.$$

Observation 1.2. *If P_n is the path graph with n vertices, the Trinajstić index is equal to*

$$NT(P_n) = 2\binom{n+1}{4}.$$

Observation 1.3. *For a complete graph K_n and a cycle graph C_n the Trinajstić index is equal to 0.*

2. Quality of Trinajstić index

Many papers are dealing with the "quality of topological descriptors". This is a vague term, which is viewed and defined differently by many researchers. There were attempts to unify these approaches and to gather a set of requirements that a novel topological invariant should fulfill. One of the best known in the circles of chemical graph theorists, and commonly quoted, is the Randić set of qualities that a novel topological descriptor should possess [15]. There, Randić compiled a list of thirteen tests to which a novel topological index should be subjected. If it would successfully pass these tests, then it would be qualified for further and deeper investigations. Some of these tests are of pure chemical nature, while some of them are technical, which almost all topological indices fulfill. These tests will be omitted. Here, the results of the two most important structural tests of the Trinajstić index will be presented and compared with other similar topological descriptors.

2.1. Correlations with other descriptors

Reasons for introducing novel topological indices, which are highly correlated with other similar indices, are quite difficult to understand because almost all structural features of the underlying graph can be harvested with the already existing invariants. Therefore, it is of utmost importance to check whether the correlations of a novel descriptor with other similar indices are exceeding the permitted upper limits. A bunch of indices that belong to the same type as the Trinajstić index were employed for testing relations among them. In particular, beside NT, the Wiener index (W) [18], hyper-Wiener index (WW) [14], Tratch-Stankevich-Zefirov index (TSZ) [17], hyper-Szeged index (hSz) [2], Mostar index (Mo) [4], and total-Mostar index tMo [12] were used in this investigation. These topological indices were calculated for all trees with 10 vertices, and obtained correlations are given in the Figure 1. The Szeged index and the revised Szeged index weren't included in these tests because their values coincide with the Wiener index in the case of trees.

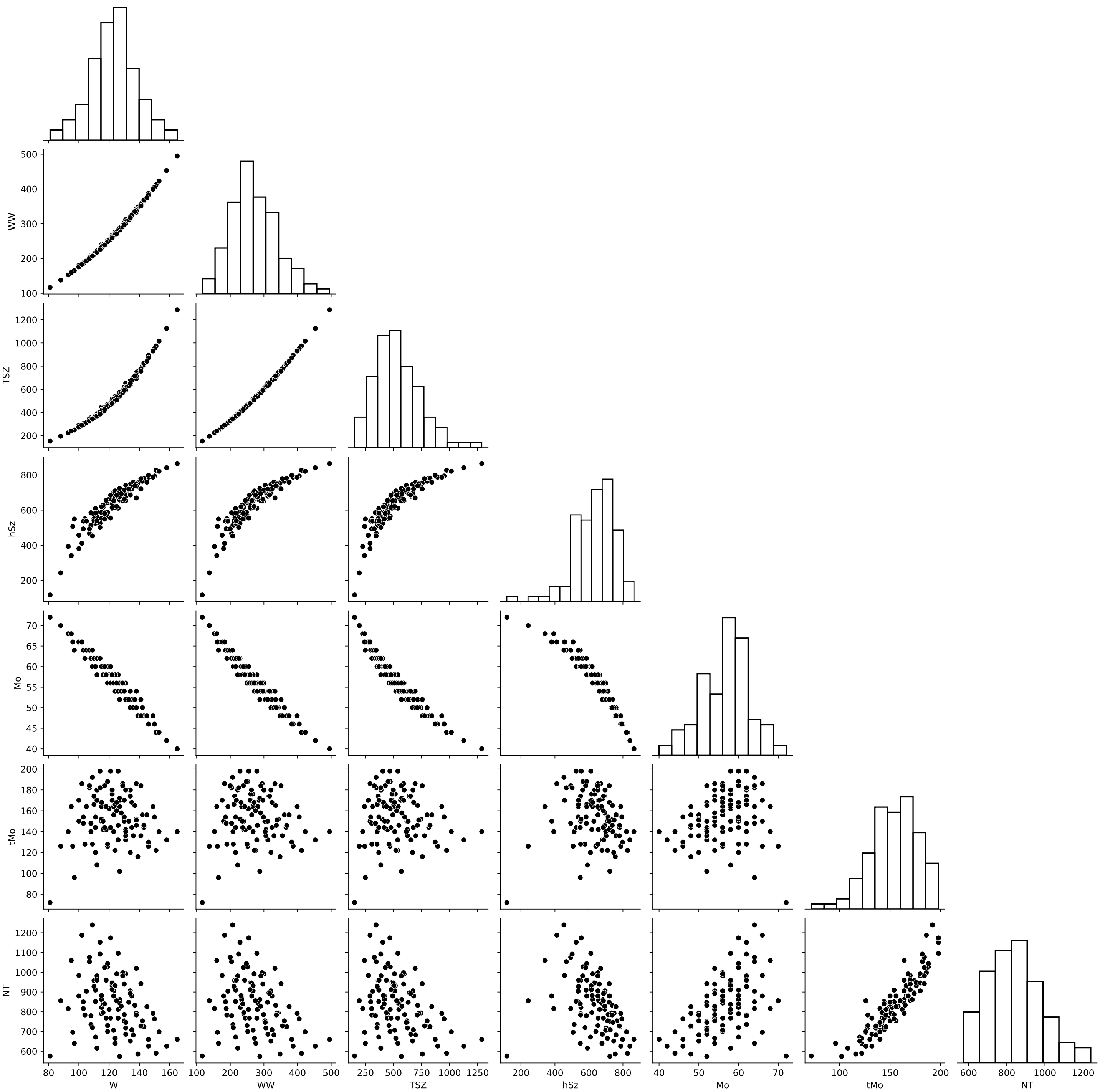

Figure 1: Correlations among Trinajstić, Wiener, hyper-Wiener, Tratch-Stankevich-Zefirov, hyper-Szeged index, Mostar, and total-Mostar indices.

It is evident from Figure 1 (see last row of the figure) that the Trinajstić index is loosely correlated only with the total-

Mostar index, and there is no detected correlations with other indices. The correlation coefficient between the NT and tMo is 0.902. The correlation graph is given in Figure 2, where the vertices are the topological indices, and an edge connecting two vertices is added if the correlation coefficient between them is greater than 0.9. The higher the absolute value of the correlation coefficient, the thicker edge in Figure 2.

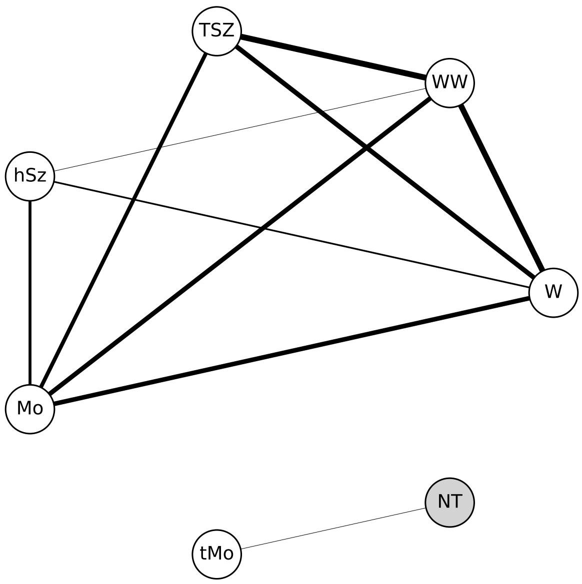

Figure 2: Correlation graph.

This test is supporting the introduction of the Trinajstić index, because the obtained correlations indicate that NT gathers rather different structural details than other topological indices, employed in this investigation.

2.2. Degeneracy of Trinajstić index

The most desirable quality of a topological index would be complete discrimination among all graphs, or at least among all isomers. Unfortunately, such a "divine property" of a descriptor is unreachable even today. Thus, topological indices should be tested and ranked also according to their discrimination power. A method for assessing the degeneracy (a.k.a. discrimination power) of a topological index is introduced and clearly explained in [10]. The degeneracy of the Trinajstić index and all other indices that are listed in Subsection 2.1 were calculated using the set of all trees with 10 vertices. The results are given in the Figure 3 and the Table 1.

Topological index	% of degeneracy
NT	19.81
Mo	83.96
tMo	62.26
hSz	18.87
W	50.00
WW	14.15
TSZ	8.49

Table 1: The percent of degeneracy of listed topological indices, calculated on the set of trees with 10 vertices.

It is evident that the Trinajstić index belongs to the set of indices with a reasonably low degeneracy. It is somewhat surprising that its relatives, such as the Mostar and the total-Mostar indices, have such a high extent of degeneracy.

3. Extremal graphs

A quest for graphs with the extremal values of a topological index is one of the primary mathematical investigations that need to be done. Here, the conjectures for extremal graphs in the case of trees and all connected graphs will be listed. These conjectures are based on extensive computational investigations. All calculations were performed on a home computer and

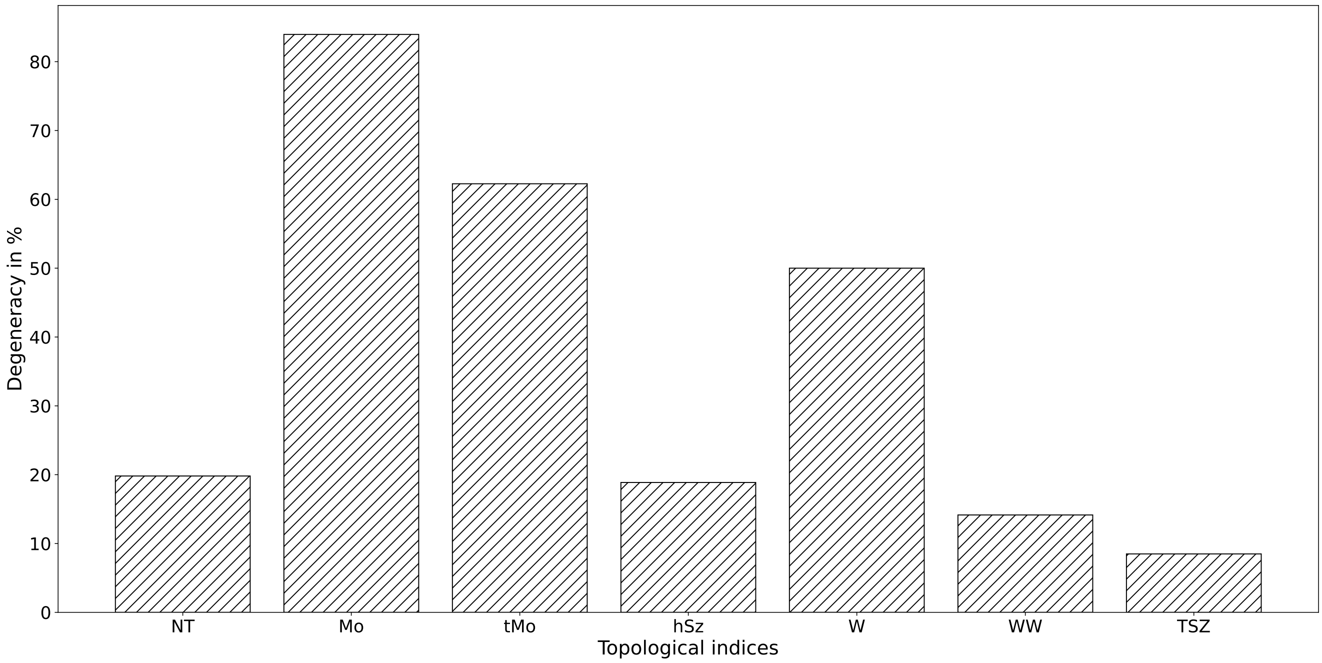

Figure 3: The levels of degeneracies of Trinajstić (NT), Mostar (Mo), total-Mostar (tMo), hyper-Szeged index (hSz), Wiener (W), hyper-Wiener (WW), Tratch-Stankevich-Zefirov (TSZ) indices.

all programs have been coded in Python 3.8 using NetworkX module [8]. The datasets of graphs were generated by the nauty generators [11].

Trees

To be able to draw some conclusions and establish some conjectures on trees with extremal Trinajstić index, the screening, by brute-force method, were performed on the classes of graphs from 6 to 20 vertices. The obtained results led to the following conjecture:

Conjecture 3.1. *For trees with order greater than 10 vertices, the star graph has the minimal value of the Trinajstić index.*

Trees, having the minimal NT with the order up to 10 vertices are given in the Figure 4.

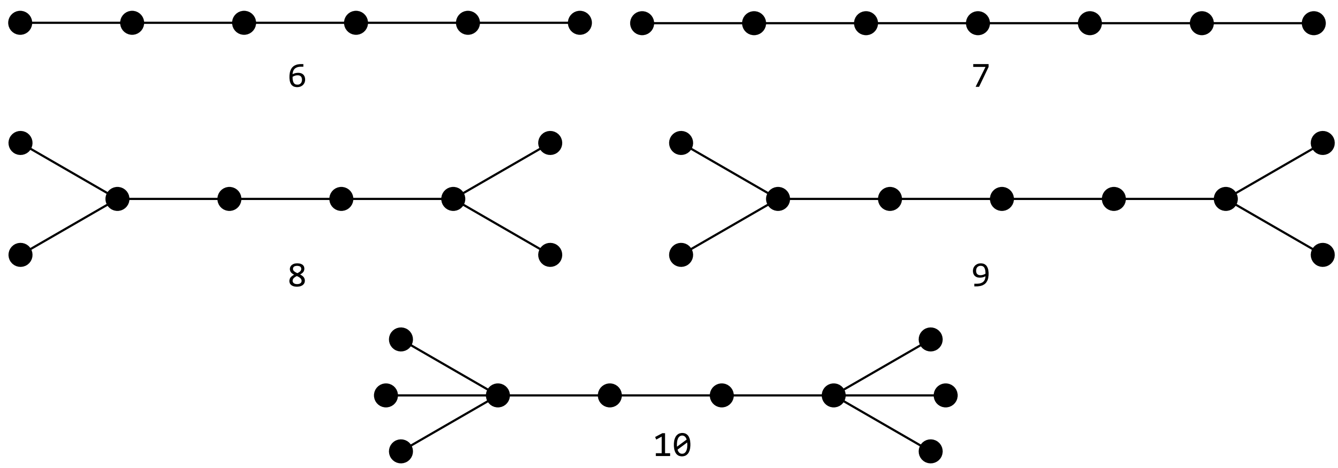

Figure 4: Trees with the maximal Trinajstić index.

Characterization of trees with the maximal Trinajstić index is far from a task that is easy to be done. However, based on the extensive computation, a couple of features of a tree with the maximal NT can be detected. Firstly, the tree which maximizes the Trinajstić index has the central vertex whose degree is greater than 2. All other vertices are of degree 1 or 2. In other words, the NT-maximal tree has the central (root) vertex to which are attached several paths of a rather small length. We considered in this search the trees with the order up to 20 vertices. As it can be seen in Figure 5, the length of paths is limited to 3, but it can be expected that in the case of larger trees, the length of paths will increase. Additionally, it should be noted that (except in the case of trees with 6 vertices) there is always a unique NT-maximal tree with given order.

Author of this article did not succeeded to characterize the tree that maximizes the Trinajstić index. The NT-maximal trees from 6 to 20 vertices are depicted in Figure 5.

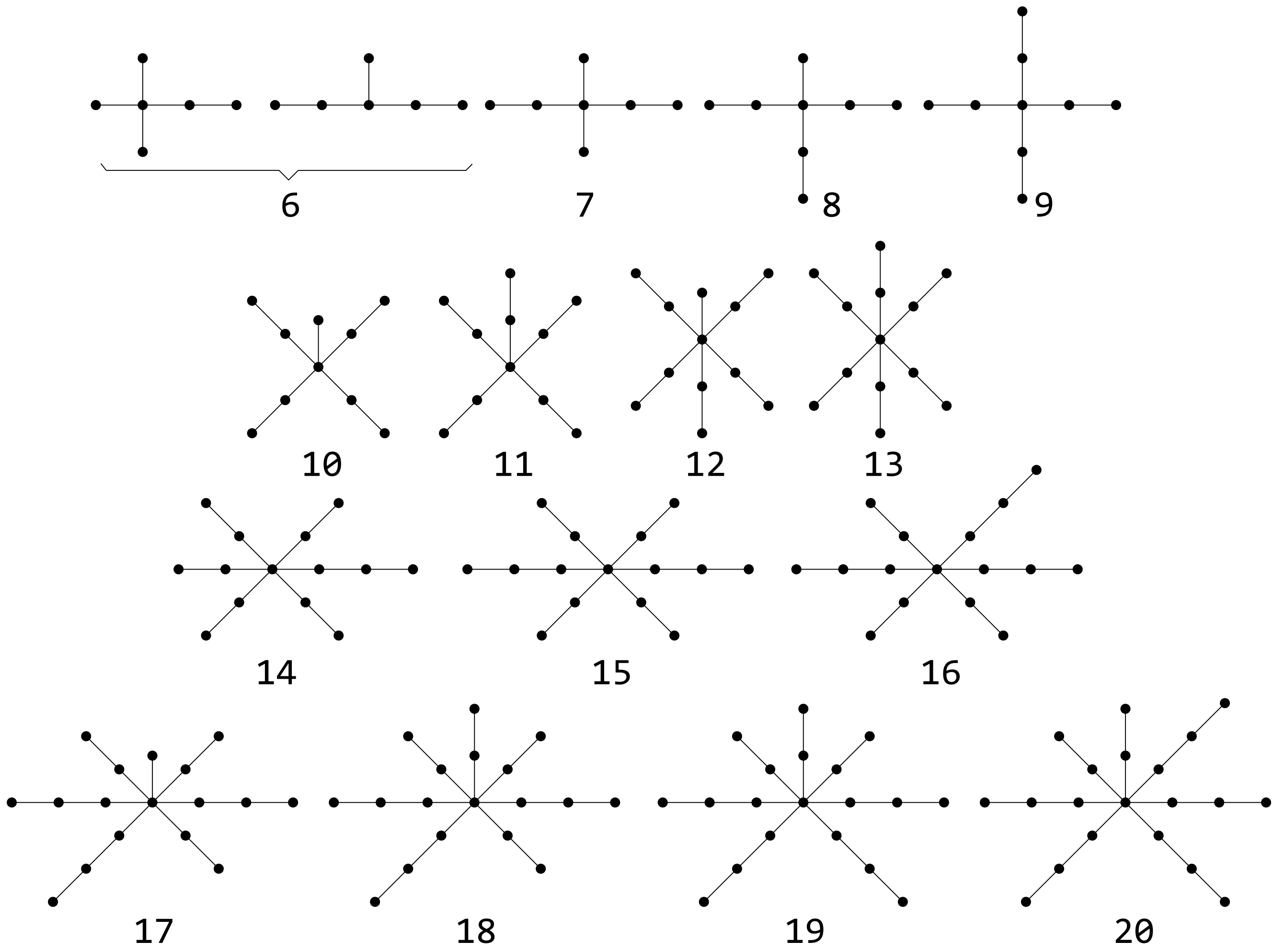

Figure 5: Trees from 6 to 20 vertices having the highest value of the Trinajstić index among isomeric trees.

Connected graphs

The following conjectures are based on the brute-force computing approach in pursuing connected graphs with minimal and maximal Trinajstić index. This type of scanning was done for all connected graphs from 5 to 10 vertices.

Since the Trinajstić index is another measure of unbalancedness, its value for the totally balance graphs is equal to 0. Thus, it was already detected that the cycle and the complete graphs have 0 value for this index. Taking this into the mind and the results obtained from computer searching, the following conjecture about graphs with minimum Trinajstić index can be composed:

Conjecture 3.2. *The minimum value of the Trinajstić index is equal to 0. The necessary but not sufficient condition for a graph to reach the minimum of the Trinajstić index is to be a regular graph.*

As for the graph that maximizes the Trinajstić index, the computationally obtained results suggest the following:

Conjecture 3.3. *The graph with the maximal value of the Trinajstić index is unique. It is consisting of a complete subgraph* $K_{\lceil n/2 \rceil}$*, on whose vertices are attached* $\lfloor n/2 \rfloor$ *pendent vertices. One pendent vertex is allowed per vertex that belongs to the complete subgraph.*

4. Conclusion

The newly proposed Trinajstić index was subjected to several tests that justified its introduction. This index belongs to the class of measures of unbalancedness. Several mathematical conjectures, based on the extensive computer searching, were put forward. It is believed that the Trinajstić index could be a potentially useful topological invariant in the field of chemical graph theory.

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