Important Mathematical Structures of the Topological Index *Z* for Tree Graphs†

Haruo Hosoya*

Ochanomizu University (Emeritus), Bunkyo-ku, Tokyo 112-8610, Japan

Received October 31, 2006

Mathematical importance of the topological index, Z_G, or the so-called Hosoya index is stressed by presenting and giving supporting evidence for the proposed conjecture. That is, for a given pair of positive integers ($n_1<n_2$) which are prime with each other there exists a series of Z-trees $\{G_m\}$ of the property, $Z(G_m) = Z(G_{m-1}) + Z(G_{m-2})$ ($m\geq 3$), with $Z(G_1) = n_1$ and $Z(G_2) = n_2$.

INTRODUCTION

Triggered by the debut of the *Z*-index in 1971 a number of topological indices have been proposed not only for QSAR or QSPR studies in chemistry but also for characterizing the topological structure of graphs in mathematics.[1−4] From the standpoint of practical chemistry proper combination of several topological indices usually gives better correlation than any other single topological index. However, the more the number of indices is increased, the more physico-chemical interpretation of the property concerned would be diluted. In this situation the *Z*-index has a peculiar property than any other topological indices ever proposed. Namely, although various applications to chemical problems have been explored through the *Z*-index,[5−9] its mathematical meaning is the clearest among the big family of topological indices.[10]

Since the *Z* index has repeatedly been introduced in the literature,[1−10] only its least account will be given here. For the sake of simplicity, consider here a structural formula of a saturated hydrocarbon molecule, say *n*-butane or butadiene. By deleting all the H atoms and changing the remaining C atoms into vertices, one can obtain the chemical graph (G) or a path graph S_4 in the graph theory, which is composed of four vertices and three consecutive edges. If one defines the non-adjacent number, $p(G,k)$, as the number of ways for choosing k disjoint edges from G, we have $p(G,1) = 3$ (number of edges in G). As one can choose a pair of (disjoint) double bonds for drawing the Kekulé structure of butadiene, $p(G,2) = 1$ is obtained for S_4. For any graph $p(G,0)$ is defined to be unity. The topological index Z_G for G is defined to be the sum of all the $p(G,k)$ numbers for G as

$$Z_G = \sum_{k=0}^{m} p(G,k) \tag{1}$$

As $p(G,k) = 0$ for $k > 2$ in S_4, its Z_G is obtained to be $1 + 3 + 1 = 5$. In Table 1 the *Z*-indices of smaller members of path graphs, $\{S_n\}$, or the chemical graphs for linear polyenes or normal alkanes are given. In this case the topological indices of the series of S_n graphs are shown to form the famous Fibonacci numbers which obey the following recursive relation

Table 1. $p(G,k)$ and Z Values of Path Graphs $\{S_n\}$ or the Carbon Atom Skeletons of Linear Polyenes and Normal Alkanes

		$p(G,k)$ [a]				
n	G (S_n)	$k=$ 0	1	2	3	Z_G (F_n) [b]
1		1				1
2		1	1			2
3		1	2			3
4		1	3	1		5
5		1	4	3		8
6		1	5	6	1	13
7		1	6	10	4	21

[a] Note that $p(S_n,k) = \binom{n-k}{k}$. [b] The initial values (F_0=F_1=1) of the Fibonacci numbers in this paper are different from the conventional definition.

$$Z(S_n) = Z(S_{n-1}) + Z(S_{n-2}) \tag{2}$$

Especially for tree graphs, or the carbon atom skeleton of acyclic hydrocarbon molecules, the *Z*-index can also be obtained by adding the absolute values of the coefficients of the characteristic polynomial of a given graph.[1] Trinajstic has demonstrated a number of chemical problems where the characteristic polynomial of a graph is involved.[2] One of the most important issues in these problems is Sachs's theorem,[11] which has a very important role for interpreting and explaining the mathematical meaning of *Z*.

The *Z*-index was shown to be well correlated with many thermodynamic quantities, such as boiling point, and also with Hückel molecular orbital quantities, such as total π-electron energy and bond orders.[1−10]

† Dedicated to Professor Nenad Trinajstić on the occasion of his 70th birthday.

* Corresponding author e-mail: hosoya@is.ocha.ac.jp.

10.1021/ci6004756 CCC: \$37.00
Published on Web 05/11/2007

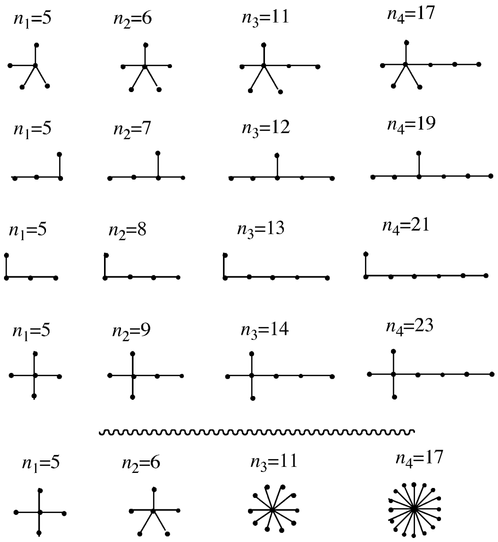


Figure 1. 1. Illustrative examples of the conjecture to be discussed in this paper for the cases with $n_1 = 5$ and $n_2 = 6-9$. The series of star graphs in the bottom row are trivial and not discussed in this paper.

On the other hand, it was gradually becoming clear that the Z-index has a key role in analyzing and interpreting the mathematical structure of a number of elementary mathematics and algebraic number theory, such as Pascal's, Pythagorean, and Heronian triangles, Fibonacci, Lucas, and Pell numbers, and Pell equations.[12,13] In some cases the Z-index is shown to be used as a powerful proof technique.

Recently the present author proposed the following conjecture.[13]

Given a pair of positive integers, $n_1 < n_2$, which are prime with each other, there exists a series of graphs, $\{G_n\}$, so that their Z-indices have the Fibonacci-type property (2), i.e.,

$$Z(G_1) = n_1,\ Z(G_2) = n_2 \quad \text{and} \quad Z(G_m) = Z(G_{m-1}) + Z(G_{m-2})\ (m \geq 3)$$

Examples are given in Figure 1, where n_1 is given to be fixed at 5. The integer n_2 is supposed to be larger than n_1. So first try to choose 6 for n_2. Then one can draw the series of graphs in the top row, whose Z-values have the desired property as above. One can continue to grow them by extending the longest branch edge-by-edge to the right. Similarly by choosing 7−9 for n_2 one can draw a different series of regularly growing tree graphs with the common recursive property but with different initial conditions as shown, respectively, in the second to fourth rows.

There exist two different tree graphs with $Z = 5$. As will be shown later in Figure 7 there are four distinctive vertices among this pair of tree graphs. Note that all four n_2-graphs appearing in Figure 1 grew up from either of the two n_1-graphs by attaching a unit edge at one of the above four distinctive vertices. How about the case with n_2 larger than 9? As 10 is a multiple of 5, the problem is reduced to the case with $n_1 = 1$ and $n_2 = 2$. As will actually be demonstrated later (see Figure 10), for any n_2 larger than 11 and prime to 5 one can prepare a series of regularly growing tree graphs with the Fibonacci-type recursive property.

It is to be remarked here that a series of star graphs with this property always exists for any pair of integers as shown in the bottom of Figure 1. A star graph $K_{1,n}$ is a tree composed of a center vertex and n edges emanating from it, and its Z-value is $n+1$. However, this solution is trivial, because no mathematically meaningful information or no practically useful consequence is derived from it, and thus we will no longer treat this type of solution in this paper. On the other hand, the existence of all other series of graphs in Figure 1 has a very important mathematical meaning as follows.

Namely, any algebraic discussion using some Fibonacci-type recursion relation can be translated into geometry (in graph-theoretical sense) or interpreted by geometrical objects. As a result perspective discussion spanning both the algebraic and geometrical worlds can be possible not only for interpreting and relating the existing theories but also for constructing quite new ones. However, it is very difficult to gain a general proof of this conjecture in a purely mathematical way. Thus the purpose of the present paper is to provide as many facts as possible for supporting this conjecture.

PROPOSITION OF THE CONJECTURE

When the conjecture was first proposed, nontree graphs were implicitly involved. However, due to substantial progress in this study the present author now believes that "tree graphs" suffice here.

First let us define a few terminologies for the sake of a compact and clear-cut discussion. The "*Zn*-graph" (n: natural number) is a graph whose Z-index is n. The Z-graph is its generic name and is usually meant to involve various *Zn*-graphs. When the graphs are limited to tree graphs, the terms *Zn*-trees and Z-trees are used. The number of *Zn*-graphs with a given n is denoted by *NZn*. Whether *NZn* is meant for general graphs or trees may be understood in the context. For example, as there are a pair of Z5-trees, + and −•−•−, one may well say that *NZ*5 is two.

Then the above-mentioned conjecture can be paraphrased as follows.

Conjecture: For a given pair of natural numbers, $n_1 < n_2$, which are prime with each other, there exists a series of regularly growing Z-trees $\{G_m\}$ of the property, $Z(G_m) = Z(G_{m-1}) + Z(G_{m-2})$ $(m \geq 3)$, with $Z(G_1) = n_1$ and $Z(G_2) = n_2$.

As stated before, it is very difficult to accomplish a general proof of this conjecture in purely mathematical way. Then let us start step by step from the beginning.

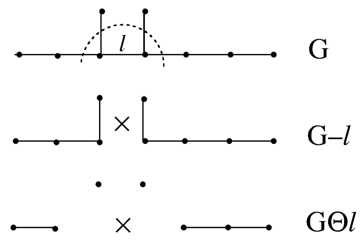
Z-INDEX AND ITS RECURSIVE RELATION[1]

As already shown in Table 1, the Z-indices of path graphs $\{S_n\}$ obey the Fibonacci-type recursive relation (2). If the initial values for the Fibonacci numbers are chosen as

$$F_0 = F_1 = 1 \tag{3}$$

contrary to the conventional one ($F_1 = F_2 = 1$),[14,15] we have a beautiful relation

$$Z(S_n) = F_n \tag{4}$$



$$Z(\mathrm{G}) = Z(\mathrm{G}-l) + Z(\mathrm{G}\Theta l)$$
$$= Z(\mathrm{S}_4)\, Z(\mathrm{S}_5) + \{Z(\mathrm{S}_1)\}^2\, Z(\mathrm{S}_2)\, Z(\mathrm{S}_3)$$
$$= 5 \times 8 + 1 \times 1 \times 2 \times 3$$
$$= 46$$

$$p(\mathrm{G},k) = p(\mathrm{G}-l,k) + p(\mathrm{G}\Theta l,k-1)$$

Figure 2. 2. An example of application of recursion formula for obtaining the Z-index of a branched tree graph. By deleting edge l from G one gets subgraph G−l composed of two disjoint components, the product of whose Z-values gives Z(G−l). Further by deleting all the edges which were incident to l one gets GΘ l with four components in this case. Since all the components of G−l and GΘ l belong to S_n, one can calculate Z(G) by using the Fibonacci numbers given in Table 1.

For a tree graph composed of n vertices the characteristic polynomial, $\mathrm{P_G}(x)$, which is defined in terms of the $n \times n$ adjacency matrix $\boldsymbol{A}$ and unit matrix $\boldsymbol{E}$ as

$$\mathrm{P_G}(x) = (-1)^n \det(\boldsymbol{A} - x\boldsymbol{E}) \tag{5}$$

can be obtained just by using the set of p(G,k)'s as follows:[1,16]

$$\mathrm{P_G}(x) = \sum_{k=0}^{[n/2]} (-1)^k\, p(\mathrm{G},k)\, x^{n-2k} \tag{6}$$

This relation can be derived directly from Sach's theorem for the case where the graph is a tree.[11] We are not going into detail here, but $\mathrm{P_G}(x)$ for a nontree graph can also be obtained by expanding eq 6 with proper correction terms for the ring contribution.[16]

The p(G,k) and Z(G) values for larger and more complicated graphs can be obtained by using their recursive relations. Namely, by choosing an edge l from G the recursive relations for p(G,k) and Z(G) are given by[1,6,8,10]

$$p(\mathrm{G},k) = p(\mathrm{G}-l,k) + p(\mathrm{G}\Theta l,k-1) \tag{7}$$

and

$$Z(\mathrm{G}) = Z(\mathrm{G}-l) + Z(\mathrm{G}\Theta l) \tag{8}$$

where G−l is the subgraph of G obtained by deleting l, whereas GΘl is obtained from G−l by deleting all the edges which *were* incident to l in G (see Figure 2). These relations can be derived from the inclusion−exclusion principle.[17,18]

For later discussion the vertices of tree graphs are classified into the following types (see Figure 3). The *tip* vertex (t) is a vertex whose degree is unity. The only neighbor of a given (t) is called *junction* (j) but can be classified into two, *outer junction* (o) and *inner junction* (i) depending on the sizes of the components of GΘj as will be explained below, where GΘj is the subgraph of G obtained by deleting (j) together with all the edges incident to (j).

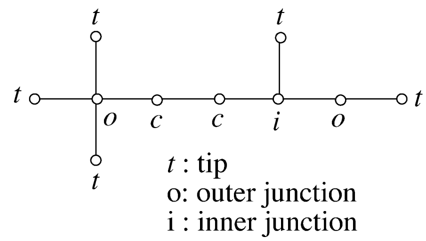


Figure 3. 3. Classification of vertices of tree graphs. See text for explanation.

Let us consider here a nonstar tree graph G as exemplified in Figure 3. By deleting a (j) vertex from G, the resultant GΘj has more than two components. If there is only one component whose vertex number is larger than two and all other components are isolated vertices, then this (j) vertex belongs to (o). On the other hand, if there are two or more components of GΘj whose vertex numbers are larger than two, (j) belongs to (i). The vertex which does not belong to any of the above types is called *core* vertex (c) whose topological distance to any (t) is at least two.

A star graph or an n-star graph $\mathrm{K}_{1,n}$ is composed of n(t) vertices and the central vertex of (o), although in this case all the components of GΘj are isolated vertices. For smaller trees with $n < 6$ all the (j) vertices belong to (o), as will be shown later. Anyway distinction between (o) and (i) is important in the following discussion.

Although at the present stage the conjecture cannot yet rigorously be proved, the chain or network of logic for attacking this problem has been set up. The strategy is as follows.

STRATEGY FOR PROVING THE CONJECTURE

First the three steps for proving the conjecture are given irrespective of the fact that they have been proved or not.

(i) If tree graph G_1 is given, one can obtain a series of Z-trees $\{\mathrm{G}_m\}$ with the following recursive property

$$(\#1)\ Z(\mathrm{G}_m) = Z(\mathrm{G}_{m-1}) + Z(\mathrm{G}_{m-2})\ (m \geq 3)$$

by extending a branch from any vertex v in G_1. Let us call such a v 'bud'.

(ii) If a positive integer n_1 is given, one can obtain a pair of Zn_1- and Zn_2-trees for any n_2 (or m) under the following condition

$$(\#2)\ n_1 < n_2 = n_1 + m < 2n_1 \quad \text{and} \quad (n_1, n_2) = 1$$

where the expression (n_1, n_2) denotes the greatest common measure (GCM) of the pair of integers, n_1 and n_2. Then the latter condition means that n_1 and n_2 are prime with each other.

As will be explained later, this statement asserts that one can find a bud vertex v in one (G) of the Zn_1-trees with $Z(\mathrm{G}\Theta\mathrm{v}) = m$ under condition (#2). Namely

$$(\#2')\ 0 < m < n_1 \quad \text{and} \quad (n_1, m) = 1$$

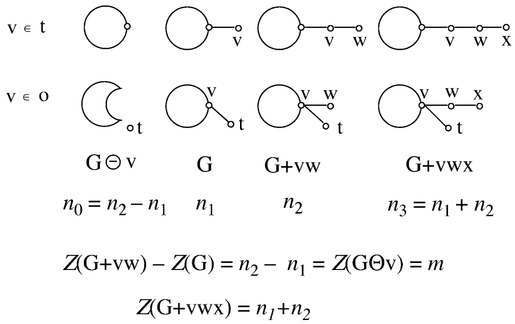


Figure 4. 4. Relation among the *Z*-indices of a series of graphs derived by growing of a branch from bud vertices of (t) and (o) types.

(iii) If a pair of Zn_1- and Zn_2-trees satisfying condition (#2) or (#2′) are given, one can obtain a series of Zn_2-trees under the following condition

$$(\#3)\ n_1 < n_2 = kn_1 + m\ (k \geq 2) \text{ and } (n_1, n_2) = 1$$

and the conjecture is proved.

As will be shown, step (i) is quite easy to prove. Step (iii) can also be proven. Thus our main target is to prove step (ii).

PROOFS AND VERIFICATION

Proof of Step (i). Although there are four different types of vertices in tree graphs, first consider the cases with (t) and (o) types for choosing a proper bud vertex. See Figure 4, where two sets of graphs, GΘv, G, G+vw, and G+vwx, for v = (t) and (o) are shown. In either case a branch is growing from the bud vertex v of G to w and x. For proving step (i) GΘv is unnecessary. Namely, by applying the recursive relation 8 to the edge wx of G+vwx, $n_3 = Z$(G+vwx) becomes equal to the sum of $n_2 = Z$(G+vw) and $n_1 = Z$(G) for any type of v. For the case with v∈tGΘv is a connected graph, and it can be accommodated into the family of {G_m} satisfying (#1). For the case with v[element]o the graph GΘv becomes disconnected, but one can discard all the isolated vertex or vertices from the components of GΘv, as those *Z*-indices are unity. Then in this case also the largest component of GΘv can be accommodated into the family of {G_m}.

However, for the cases with v∈i and c there arise more than two components for GΘv whose *Z*-values are larger than 2. Then those graphs cannot be accommodated into the family of {G_m}. Thus these two cases will no longer be considered.

Supplementary Remark to Step (ii). As already noticed in the above section, the increment, Δ, of *Z*(G) caused by growing G into G+vw by attaching a unit edge vw to v (see Figure 4) is equal to *Z*(GΘv)

$$m = Z(\mathrm{G{+}vw}) - Z(\mathrm{G}) = Z(\mathrm{G\Theta v}) = n_2 - n_1 < n_1$$

owing to eq 8. Then our target becomes what is stated in the latter part of (ii).

Namely, it has to be checked if one can select a set of bud v's from G so that the values of *Z*(GΘv) = *m* span all such integers from 1 to n_1-1 that are prime to n_1. As will be shown later, in all the cases in Figures 5−8 one can select such complete sets of bud v's by choosing only from (t) and (o) vertices. Further, although this important property could not be proved yet, at least up to $n_1 = 75$ no violation to this rule has been observed.

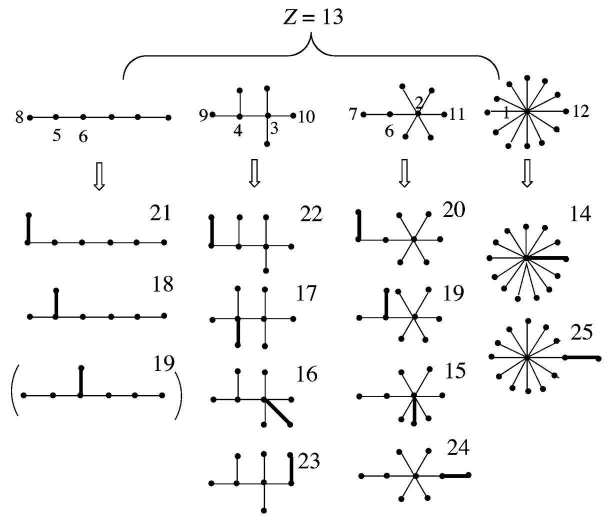


Figure 5. 5. Diagram showing that all the tree graphs of *Z* = 14−25 can be generated from the set of *Z*13-trees by using their *Z*(GΘv) values (small figures). By attaching a unit edge at one of the distinctive edges of the four *Z*13-trees one gets various n_2-graphs with *Z* ranging from 14 to 25. The *Z*19-tree in parentheses which grew up from a vertex of (c)-type is redundant and unnecessary.

Before demonstrating the actual examples let us remark about the factorable property of the *Z*-index.

***Zn*-Trees of Prime and Composite Numbers.** The present author has pointed out that the numbers of Kekulé structures for highly symmetrical polycyclic aromatic hydrocarbons are usually highly factorable and vice versa.[19] On the other hand, such a difference is not so clear for the *Z*-index. However, as will be shown later it is a general tendency that the *Z*-graphs for prime *Z*'s are less symmetrical than those for *Z*'s of composite numbers.

Contrary to this observation it is definitely true that *NZn* for prime *n* is larger than that for *n* ± 1 only with a few exceptions. Our task is to find the *Z*-trees corresponding to any pair of integers, n_1 and n_2, which are prime with each other so that the recursive relation (#1) as in the situation of Figure 4 is fulfilled. Thus the factorable property of integers is one of the most crucial issues in the present analysis.

Verification of Step (ii). First try to consider the case with $n_1 = 13$ as a typical prime number.[20] As seen in the top row of Figure 5 there are four *Z*13-trees, which in total have 13 distinct vertices (v's). The number (printed in small figure) assigned to each v is *Z*(GΘv), which exactly gives the increment, *m*, of *Z*(G) caused by growing G into G+vw by attaching a unit edge vw to v as already shown in Figure 4.

Note that in Figure 5 the *Z*(GΘv) values run consecutively from 1 to 12 with only a pair of redundancy at 6, and one may discard the vertex of (i) type in the leftmost tree yielding the *Z*19-tree, which are parenthesized. Thus in the case with $n_1 = 13$ one could prepare a complete set of *Z*-graphs having the recursive property of (#1) for any n_2 fulfilling the condition (#2) just by selecting bud v's only from (t) and (o) types. Those Zn_2-trees (with larger figures of n_2 from 14 to 25) are also shown in Figure 5.

Next consider the cases with $n_1 = 12$ and 14, both of which are composite numbers. As seen in Figure 6, both the *NZ*12

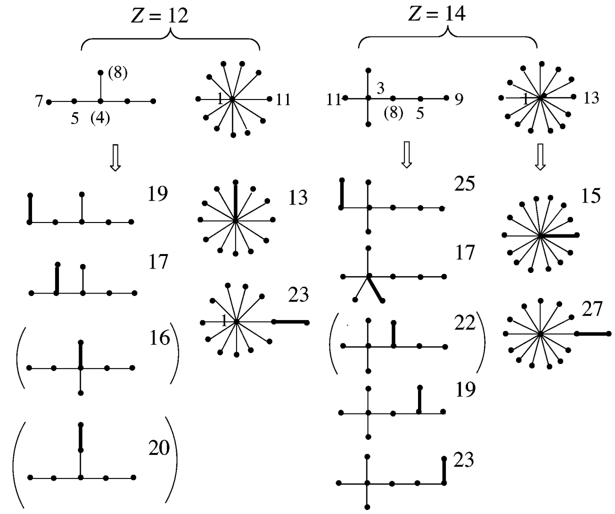


Figure 6. 6. Tree generation from the sets of Z12- and Z14-trees. The trees in parentheses are unnecessary.

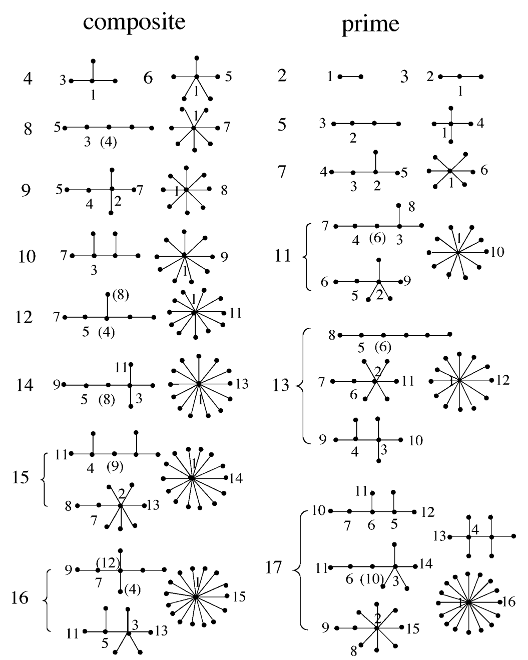


Figure 7. 7. Z(GΘv) values for Zn-trees of smaller n from 2 to 17. NZn's for composite numbers are generally smaller than those for prime numbers. Consult also Figure 1 and its explanation.

and NZ14 are two. The numbers smaller than and prime to 12 are 5, 7, and 11, while for $n_1 = 14$ we have $m = 3, 5, 9, 11$, and 13. In this analysis 1 should be included in the group of m's under condition (#2), and it is found to be available from the v's of (t) and (o) types in each set of Zn-trees. Those numbers are surely included in the sets of Z(GΘv) values for their respective Zn-trees. Then for the case with $n_1 = 12$ one can obtain the Z-trees with $n_2 = 13, 17, 19$, and 23, and for $n_1 = 14$ we have $n_2 = 15, 17, 19, 23, 25$, and 27. Those Zn-trees which are unnecessary in this analysis are put into a pair of round brackets. Again notice that in both cases in Figure 7 one can construct a complete set of Zn_2-trees fulfilling the conditions (#1) and (#2) by selecting the bud v's of only (t) and (o) types.

Now we have observed the following facts. (1) NZn for prime number n is larger than those for $n \pm 1$. (2) The number of distinct Z(GΘv) values for a prime number is relatively larger than those for composite numbers nearby.

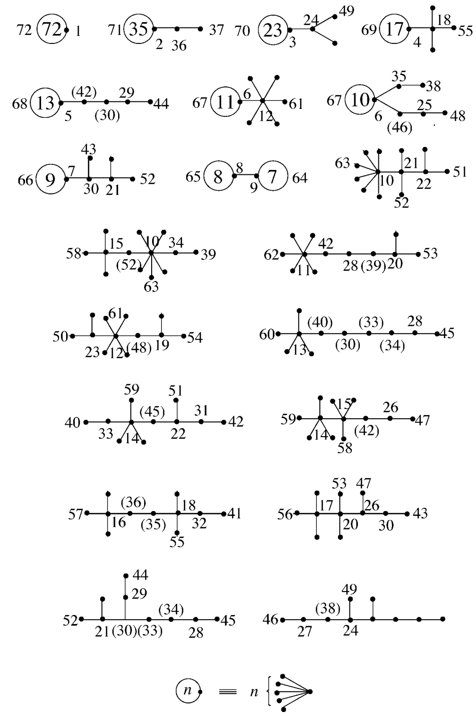


Figure 8. 8. Z(GΘv) values for Z73-trees. The number n in a circle indicates the number of edges of star graph $K_{1,n}$.

(3) Z(GΘv) values of Zn-trees for prime n seem to distribute smoothly from 1 to $n-1$. (4) For composite number n the Z(GΘv) values do not span all the numbers from 1 to $n - 1$ but seem to cover all the numbers which are prime to n. (5) One can choose only the vertices of (t) and (o) types for selecting buds in (3) and (4). (6) The sum of Z(GΘv) values for every pair of (t) and (o) vertices forming a terminal edge is equal to the Z-value of the parent tree.

The above observations can be assured by careful observation of Figure 7, where Z(GΘv) values for Zn-trees of smaller n from 2 to 17 are given. If one wants to extend this process to Z18-trees, try to choose those pairs of n_1 (the larger figure in Figure 7) and GΘv (the smaller figure) in the same tree so that $n_1 + Z$(GΘv) is equal to 18. The result is $17 + 1$, $13 + 5$, and $11 + 7$, giving three Z18-trees. However, the last two of them are found to be identical, and finally one gets a pair of Z18-trees, which give a set of Z(GΘv) = 1, 5, 7, 8, 9, 11, 13, and 17, and (#2) is shown to be fulfilled.

The proof of observation (6) has already been given implicitly in Figure 4, and this property can also be used as a good checking test for calculating the Z(GΘv) values.

We have checked up to $n_1 = 75$, and no violation to step (ii) was found. According to our experience, distribution of Z(GΘv) for a given n_1 does not seem to be random but to be governed by some deep mathematics. This inference is deduced from the careful observation of Figure 8, where Z73-trees are worked out. This is the reason why the present author believes that step (ii) is valid for any n_1.

As seen in Figure 8 NZ73 is 20. Since 73 is prime, the Z(GΘv) values were found to give all the integers from 1 to 72. The two kinds of vertices of star graph $K_{1,72}$ have the largest and smallest Z(GΘv) values. The second graph containing $K_{1,35}$ or $K_{1,36}$ as a moiety has the second largest and smallest Z(GΘv) vertices. As the size of the star graph decreases, the structure of the rest part of Zn-tree becomes complicated, and regularity ruling the Z(GΘv) values begins

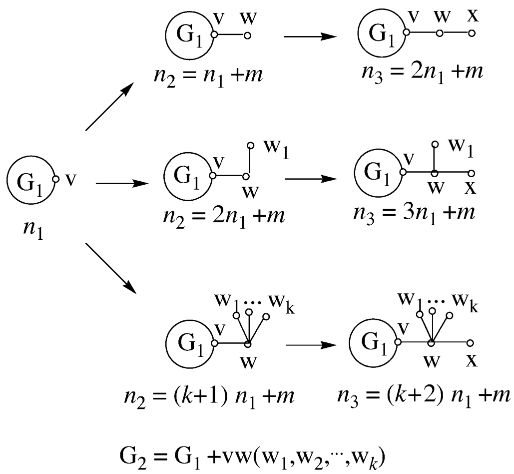


Figure 9. 9. Extension from step (ii) to step (iii). See text.

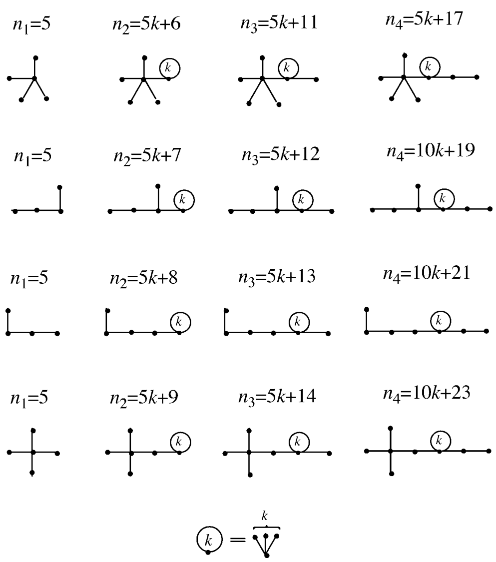


Figure 10. 10. Diagram showing that any *Zn*-tree (n>5) can be constructed as the partner of a *Z*5-tree (leftmost) generating a series of recursive *Z*-trees by growing a certain branch edge-by-edge. $k \geq 0$.

to disappear. However, besides observation (5) mentioned above it is important to notice that the ranges of the $Z(G\Theta v)$ values of (t) and (o) vertices are sharply separated as

$$1 \leq Z(G\Theta o) \leq [n_1/2] \quad [n_1/2]+1 \leq Z(G\Theta t) \leq n_1-1 \quad (7)$$

where $[n]$ is the floor function which is the largest integer not exceeding n.

Then one can enjoy finding the numbers in Figure 8 consecutively downward from 72 to 37 among (t) vertices and from 36 to 1 among (o) vertices. Of course, when n_1 is a composite number, some $\leq$ signs in observation (7) are replaced by $<$, but up to $n_1 = 75$ no exception has ever been observed.

We have thus seen how step (ii) is verified for all the cases studied. Then we will go on to the proof of step (iii) under the condition if step (ii) is true.

Proof of Step (iii). Given such a pair of positive integers n_1 and $n_2 < 2n_1$ that obey condition (#2), and suppose if a pair of Zn_1- and Zn_2-trees, G_1 and $G_2 = G_1+vw$, and the next member of the Zn_3-tree ($G_3=G_1+vwx$) with $n_3 = n_1 + n_2$ is obtained as illustrated in the top row of Figure 9. Then

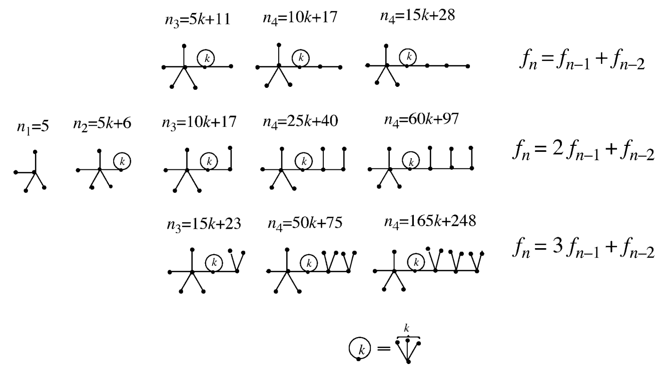


Figure 11. 11. Diagram showing the generation of a series of *Z*-trees obeying various recursive relations and starting from a *Z*5-tree. $k \geq 0$.

if another vertex w_1 is attached to w, the *Z*-value of the resultant G_2 would become $(n_1+m) + n_1 = 2n_1 + m$. Similarly by joining a set of k vertices (w_1-w_k) to w as shown in the bottom row of Figure 5 one gets the tree graph $G_2 = G_1 + vw(w_1,..., w_k)$, whose *Z*-value would become $(k+1)n_1 + m$. This means that if step (ii) is valid, the Zn_2-tree can be obtained from the Zn_1-tree for any $n_2 > n_1$ as long as $(n_1, n_2) = 1$, and the conjecture would be proved.

By using the results obtained so far, especially the information obtained from Figures 4, 7 and 9, it is easy to construct a series of *Z*-trees obeying recursive relation (#1) beginning from, for example, $n_1 = 5$. See Figure 10. For any n_2 larger than and prime to 5 one can choose the corresponding Zn_2-tree from the second column including the case with $m = 0$. The higher members of the Fibonacci-recursive property are given in the third and fourth columns of the same row.

PROSPECTIVE

We have been discussing the recursive relation of the Fibonacci type (#1). However, if our conjecture is shown to be true, we can lift up this recursive relation to the form of

$$f_n = a\, f_{n-1} + f_{n-2} \quad (a\text{: positive integer}) \qquad (9)$$

By using the diagram given in Figure 11 for the case with $n_1 = 5$ it is straightforward to draw the desired *Z*-trees obeying eq 9. The present author believes that for any n_1 one can similarly construct a series of *Z*-trees obeying recursive relation 9 as an extension of the conjecture discussed in this paper.

In this way many problems in elementary algebra can be translated into or interpreted by geometry or graph theory through the *Z*-index. The important role of the *Z*-index not only is not limited to elementary mathematics but also will be found in sophisticated algebraic number theory.

ACKNOWLEDGMENT

The author thanks the two referees for their critical comments which were very helpful in improving the manuscript.

REFERENCES AND NOTES

(1) Hosoya, H. Topological Index. A Newly Proposed Quantity Characterizing the Topological Nature of Structural Isomers of Saturated Hydrocarbons. *Bull. Chem. Soc. Jpn*. **1971**, *44*, 2332−2339.

(2) Trinajstić, N. *Chemical Graph Theory*; CRC Press: Boca Raton, Florida, 1992.
(3) *Topological Indices and Related Descriptors in QSAR and QSPR*; Devillers, J., Balaban, A. T., Eds.; Gordon and Breach: Amsterdam, The Netherlands, 1999.
(4) Karleson, M. *Molecular Descriptors in QSAR/QSPR*; Wiley: New York, 2000.
(5) Hosoya, H. Topological Index as a Sorting Device for Coding Chemical Structures. *J. Chem. Doc*. **1972**, *12*, 181−183.
(6) Hosoya, H.; Hosoi, K. Topological Index as Applied to π-Electronic Systems. III. Mathematical Relations among Various Bond Orders. *J. Chem. Phys*. **1976**, *64*, 1065−1073.
(7) Gao, Y.-D.; Hosoya, H. Topological Index and Thermodynamic Properties. IV. Size Dependency of the Structure-Activity Correlation of Alkanes. *Bull. Chem. Soc. Jpn*. **1988**, *61*, 3093−3102.
(8) Hosoya, H.; Motoyama, A. An Effective Algorithm for Obtaining the Recursion Formulas of the Counting Polynomials in the Dimer Statistics. Application of Operator Technique on the Topological Index to 2- and 3-Dimensional Rectangular and Torus Lattices. *J. Math. Phys*. **1985**, *26*, 157−167.
(9) Hosoya, H. From How to Why. Graph-Theoretical Verification of Quantum-Mechanical Aspects of π-Electron Behaviors in Conjugated Systems. *Bull. Chem. Soc. Jpn*. **2003**, *76*, 2233−2252.
(10) Hosoya, H. Topological Index and Fibonacci Numbers with Relation to Chemistry. *Fibonacci Q*. **1973**, *11*, 255−265.
(11) Sachs, H. Beziehungen zwischen den in einem Graphen enthaltenen Kreisen und seinen characterstischen Polynom. *Publ. Math*. (*Debrecen*) **1964**, *11*, 119−134.
(12) Hosoya, H. Pell Equation. III. Graph-Theoretical Meaning of the Solutions of the Pell Equation through topological Index *Z. Nat. Sci. Rept. Ochanomizu Univ*. **2006**, *57*, 57−83.
(13) Hosoya, H. Mathematical Meaning and Importance of the Topological Index *Z. Croat. Chem. Acta* **2007**, *80*, in press.
(14) Hoggatt, V. E., Jr. *Fibonacci and Lucas Numbers*; Houghton Mifflin: New York, 1969.
(15) Koshy, T. *Fibonacci and Lucas Numbers with Applications*; Wiley: New York, 2001.
(16) Hosoya, H. Graphical Enumeration of the Coefficients of the Secular Polynomials of the Hückel Molecular Orbitals. *Theor. Chim. Acta* **1972**, *25*, 215−222.
(17) *Handbook of Discrete and Combinatorial Mathematics*; Rosen, K. H. Ed.; CRC Press: Boca Raton, Florida, 2000; p 432.
(18) Weisstein, E. W. *CRC Concise Encyclopedia of Mathematics*; Chapman & Hall/CRC Press: Boca Raton, Florida, 2003; pp 1472−1473.
(19) Hosoya, H. Matching and Symmetry of Graphs. *Comp. Math. Appl*. **1986**, *12B*, 271−290.
(20) The number 13 is dedicated to the author's good old friend, Professor Nenad Trinajstić, whose surname means 13.

CI6004756