A Concealed Property of the Topological Index *Z*

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Examination of the structure-dependence of the total π-electron energy leads to the equation $F(G,x) = \ln Z(G)$, where $F(G,x)$ is the Coulson function (of the molecular graph G) and $Z(G)$ is the corresponding topological index Z. The (positive and unique) solution of this equation is called the Z-point of G and is denoted by x_{H}. By the analysis of the Z-points of trees and chemical trees the following generally valid regularities were established: (a) Not all trees have a Z-point, but all chemical trees have a Z-point. (b) The Z-points of all chemical trees (irrespective of their size and other structural features) are nearly equal; for all chemical trees, $x_{\mathrm{H}} \approx 1.2$.

The topological index Z was proposed[1] in 1971 and soon thereafter its numerous chemical applications were demonstrated.[1–6] For details see the reviews.[7,8] The mathematical properties of the topological index were also extensively examined.[9–28] A comprehensive survey is found in a recent book.[29]

Let G be a molecular graph and let $p(G,k)$ denote the number of ways for choosing k disjoint (= mutually non-touching) edges from G, with $p(G,0)$ being defined to be unity for all graphs. Naturally $p(G,1)$ is equal to the number of edges of G. Then the topological index Z is defined as

$$Z = Z(G) = \sum_{k\geq0} p(G,k). \tag{1}$$

As early as in 1972 it was noticed[2] that Z is related to the characteristic polynomial $\Phi(x)$ of the molecular graph, which implies that there must exist some relation between Z and the total π-electron energy (E). The basic features of the relation between E and Z were established[10,30] in the 1970s, but its finer details remained obscure until quite recently.[31]

In the study of the relation between E and molecular structure, the Coulson integral formulas play a crucial role. Namely, in 1940 Coulson[32] expressed the total π-electron energy of a conjugated unsaturated hydrocarbon molecule as

$$E = E(G) = \frac{1}{\pi} \int_{-\infty}^{\infty} F(G,x)\mathrm{d}x \tag{2}$$

where the function $F(G,x)$ is defined in terms of the respective molecular graph G composed of n vertices as

$$F(G,x) = n - ix\Phi'(G,ix)/\Phi(G,ix). \tag{3}$$

The characteristic polynomial of G, $\Phi(G,x)$, is defined in terms of the adjacency matrix, $\boldsymbol{A}$, and the unit matrix, $\boldsymbol{E}$, of the same size, as

$$\Phi(G,x) = (-1)^n \det(\boldsymbol{A} - x\boldsymbol{E}). \tag{4}$$

In Eq. 3, $\Phi'(G,x)$ stands for the first derivative of $\Phi(G,x)$ and $i = \sqrt{-1}$.

Eventually, another graph-based function was discovered:[33]

$$F_1(G,x) = x^{-2} \ln |(-ix)^n \Phi(G,i/x)|, \tag{5}$$

with the analogous property

$$E = \frac{1}{\pi} \int_{-\infty}^{\infty} F_1(G,x)\mathrm{d}x. \tag{6}$$

If the graph G is acyclic, then its characteristic polynomial conforms to the relation[2]

$$\Phi(G,x) = \sum_{k\geq0} (-1)^k p(G,k)x^{n-2k} \quad (G \in \text{tree}), \tag{7}$$

which leads to the following property,

$$\Phi(G,i) = i^n Z(G) \quad (G \in \text{tree}). \tag{8}$$

Then we have

$$F_1(G,1) = \ln Z(G) \quad (G \in \text{tree}). \tag{9}$$

Relation 9 has been used as the starting point for determining the connection between the total π-electron energy and the topological index.[10,31,34] The idea was the following.[31,34] Instead of $F_1(G,x)$, such a function $F_1{}^*(G,x)$ was substituted into Eq. 6; this function $F_1{}^*(G,x)$ for near-zero x, very large x, and at $x = 1$ coincides with $F_1(G,x)$. Further, the function $F_1{}^*(G,x)$ is adjusted so that its integral can easily be calculated. Then the resultant expression becomes a reasonably good approximation for E.

If one wishes to repeat the analogous approach with the original Coulson function 3, one encounters a difficulty. Namely, a formula of the type 9 does not hold for $F(G,x)$, and there seems to be no direct relation between the topological index $Z(G)$ and the value of $F(G,x)$ at $x = 1$.

As outlined in detail in the subsequent section, the Coulson's function $F(G,x)$ becomes equal to $\ln Z(G)$ for some $x = x_{\mathrm{H}}$. If so, then the auxiliary function $F^*(G,x)$, defined as

$$F^*(G,x) = \begin{cases} n - n_0 - ax^2 & \text{for } |x| \leq x_{\mathrm{H}} \\ 2m(x+b)^{-2} & \text{for } |x| \geq x_{\mathrm{H}} \end{cases} \tag{10}$$

coincides with $F(G,x)$ for near-zero x, very large x, and at $x = x_{\mathrm{H}}$, provided that the parameters a and b are chosen as

$$a = (n - n_0 - \ln Z) x_H^{-2}; \quad b = \sqrt{2m / \ln Z} - x_H \quad (11)$$

where m is the number of edges of the graph G and n_0 is the number of its zero eigenvalues. Consequently, if one replaces $F(G, x)$ in the integral 2 by $F^*(G, x)$, the following approximate expression for the total π-electron energy is obtained:

$$E^* = \frac{2}{\pi} \left[\frac{2}{3}(n - n_0) x_H + \frac{1}{3} x_H \ln Z + \sqrt{2m \ln Z} \right]. \quad (12)$$

In view of Eq. 12, in order to fully understand the dependency of the total π-electron energy on molecular structure, we must possess some knowledge about the properties and structure-dependency of the quantity x_H, which we name "the Z-point" (of the respective molecular graph). Bearing this in mind, we have undertaken a detailed examination of the Z-points of trees and chemical trees. Some of the results obtained are remarkable. Our main findings may be summarized as follows:

(a) Not all trees have a Z-point, but all chemical trees have a Z-point.

(b) The Z-points of all chemical trees (irrespective of their size and other structural features) are nearly equal; for all chemical trees, $x_H \approx 1.2$.

The Coulson Function and Its Z-Point

Strictly speaking, the Coulson function 3 and the integral formula 2 might be applied only to molecular graphs of conjugated π-electron systems. However, the right-hand-sides of Eqs. 2 and 3 are well defined for all graphs. Recently the concept of "*eigenvalue sum*" was put forward,[35,36] which is equal to the half of the E-value, but applicable as a structure-descriptor to all molecular graphs (chemical trees in particular). More details are found elsewhere.[31] In view of this we extend our studies to all chemical trees (= trees in which no vertex degree is greater than 4) and, for comparative purposes, to all trees.

The Coulson function 3 has been known for a very long time[32] and its analytical properties were examined by many authors on many occasions. Yet a formal proof that for all graphs G, possessing at least one edge, the (real part of the) function $F(G, x)$ is bell-shaped has been offered only quite recently.[37]

In Fig. 1, the forms of the Coulson function 3 of three isomeric trees with eight vertices are shown and compared respectively with their $\ln Z$ values. They are (a) *n*-octane, (b) 2,2,3,3-tetramethylbutane, and (c) non-chemical star S_8 (See Fig. 2). Note the following equality

$$F(G, 0) = n - n_0. \quad (13)$$

(See Eq. 10 and the discussion in Ref. 31.)[34,37]

For reasons outlined above, we are interested in the value of the variable x satisfying the following equation:[28]

$$F(G, x) = \ln Z(G), \quad (14)$$

which is an analogue of formula 9.

We call the positive solution of Eq. 14 the Z-point (of molecular graph G) and denote it by x_H as shown in Fig. 1. Note that all the $F(G, x)$ curves are bell-shaped (See also the enlarged portion in Fig. 1a), and accordingly Eq. 14 has either one real positive solution ($= x_H$), or no such solution at all, as in the case of Fig. 1c. In the case of a general tree x_H need not exist (cf.
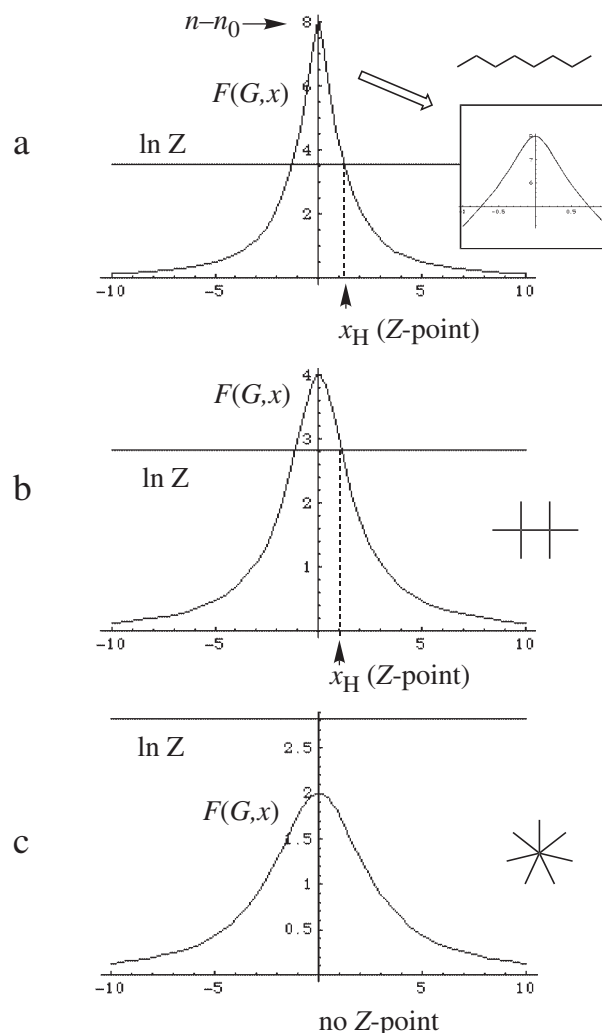

Fig. 1. Coulson's functions (Eq. 3) of (a) *n*-octane, (b) 2,2,3,3-tetramethylbutane, and (c) star S_8, compared respectively with their $\ln Z$ values. The x_H values for (a) and (b) are, respectively, maximum and minimum among the 18 octane isomers. The star graph S_8 does not have a Z-point. For (a) the curve near the origin is enlarged to show its bell-shape.
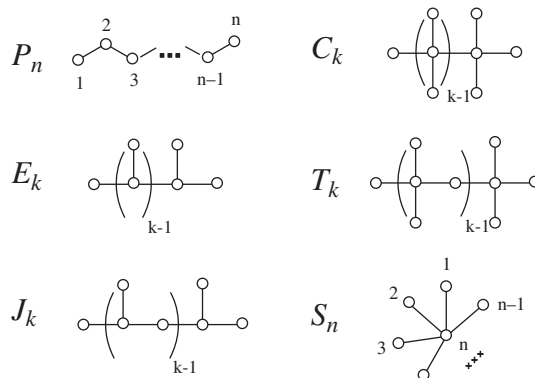

Fig. 2. Several selected series of tree graphs whose asymptotic values of x_H and r were calculated as in Table 3.

Table 1. Average, Minimal, and Maximal Values of the Z-Point of Chemical Trees with n Vertices

n	$(x_H)_{aver}$	$(x_H)_{min}$	$(x_H)_{max}$	$n.c.t.$[a]
6	1.214	1.166	1.254	5
7	1.201	1.134	1.252	9
8	1.195	1.074	1.244	18
9	1.192	0.991	1.248	35
10	1.192	1.091	1.239	75
11	1.190	1.086	1.239	159
12	1.189	1.047	1.237	355
13	1.187	0.993	1.235	802
14	1.186	1.057	1.237	1858
15	1.185	1.056	1.233	4347
16	1.185	1.032	1.234	10359
17	1.184	0.993	1.232	24894
18	1.183	1.037	1.231	60523
19	1.183	1.040	1.231	148284
20	1.182	1.022	1.229	366319

a) $n.c.t.$ is the number of distinct n-vertex chemical trees for which existence of the Z-point was examined.

Table 2. Average, Minimal, and Maximal Values of the Z-Point of Trees with n Vertices

n	$(x_H)_{aver}$	$(x_H)_{min}$	$(x_H)_{max}$	$n.t.$[a]	$n.e.$[b]
6	1.139	0.762	1.254	6	0
7	1.120	0.408	1.252	11	0
8	1.176	1.035	1.244	23	1
9	1.166	0.971	1.248	47	1
10	1.161	0.895	1.239	106	1
11	1.159	0.777	1.247	235	1
12	1.158	0.639	1.239	551	1
13	1.158	0.441	1.248	1301	1
14	1.158	0.212	1.240	3159	2
15	1.159	0.124	1.250	7741	6
16	1.159	0.285	1.243	19320	9
17	1.159	0.184	1.252	48629	11
18	1.159	0.369	1.246	123867	13
19	1.159	0.280	1.255	317955	14
20	1.158	0.162	1.249	823065	15

a) $n.t.$ is the number of distinct n-vertex trees. b) $n.e.$ is the number of trees for which the Z-point does not exist.

Table 2). Especially the star graphs S_n larger than S_8 shown in Fig. 1c do not have a real x_H value. The graph S_8 is the smallest tree graph with this property. Among the 18 chemical isomers of octane, n-octane and 2,2,3,3-tetramethylbutane, respectively, have the maximum and minimum x_H values (See Table 1). Later in this paper we prove that all chemical trees do possess a Z-point.

In order to gain information on the Z-points, their existence and structure-dependence, we computed them for all chemical trees and all trees up to 20 vertices. (Some of our preliminary results were reported in an earlier paper.[28]) In Table 1 are given the data pertaining to chemical trees and in Table 2 the analogous data for general trees.

Inspection of Table 1 shows, as a kind of surprise, that the Z-points of chemical trees are nearly constant, varying in a remarkably narrow range, and are almost completely size-inde-

pendent. Then the value $x_H = 1.2$ seems to be a reasonably good approximation for the Z-point of any chemical tree. Note that for the series of chemical trees of $n = 4k + 1$ (type T_k in Fig. 2) the value of $(x_H)_{min}$ in Table 1 rapidly converges to ca. 0.993 and is distinctively smaller than the other isomers.

From Table 2 we see that also in the case of general trees the variations in the values of the Z-point are not very large, although these are somewhat greater than in the case of chemical trees. Detailed examination reveals that the Z-points of only a few trees are exceptionally small, a phenomenon caused by the fact that for these trees $\ln Z(G)$ is only slightly smaller than $F(G,0)$, the maximum value of $F(G,x)$. For some (non-chemical) trees $\ln Z(G)$ exceeds the value of $F(G,0)$, resulting in the nonexistence of the Z-point.

Then we define the ratio r as follows for judging if a graph G has the Z-point or not:

$$r = \ln Z(G)/F(G,0). \tag{15}$$

Those graphs with r larger than 1 do not have a Z-point.

We do not possess a satisfactory theoretical explanation for the constancy of the x_H value, but we can offer a qualitative argument corroborating this regularity. According to Eq. 2, $E(G)$ is proportional to the area between $F(G,x)$ and the x-axis. Therefore x_H increases with increasing $E(G)$ (assuming that other structural parameters remain unchanged), cf. Fig. 1. On the other hand, from Fig. 1 it is evident that x_H will decrease if the value of $Z(G)$ increases (assuming that other structural parameters remain unchanged). However, it is known[10,31] that $E(G)$ is an increasing function of Z and, hence, the two effects may cancel each other.

Asymptotic Behavior of Several Series of Tree Graphs

Besides the exhaustive checking of the x_H values for all the lower members of tree graphs, asymptotic behaviors of the x_H and r values toward infinitely large graphs of several selected series shown in Fig. 2 were analyzed. In performing this analysis, the operator technique was useful for deriving the recursion formulas of the Z-index and characteristic polynomial $\Phi(G,x)$ of these larger graphs.[38] The results are summarized in Table 3, which is helpful for understanding the flow of logic in the proof of the main theorem in this paper. Note here that the behavior of the r value can rigorously be traced, while that of x_H is difficult to follow analytically.

On the Nonexistence of Z-Points

As seen from the data given in Table 2, there exist trees without a Z-point. In view of the bell-shaped form of the Coulson function (See Fig. 1), the necessary and sufficient condition for the existence of the Z-point is $F(G,0) \geq \ln Z(G)$, or $r \leq 1$. The simplest example when this inequality is violated is provided by the stars S_n for $n > 7$ (See Fig. 2). For these graphs, $p(S_n,1) = n - 1$ and $p(S_n,k) = 0$ for $k > 1$. Consequently, $Z(S_n) = n$, $F(S_n,x) = 2(n-1)/(x^2 + n - 1)$, and $F(S_n,0) = 2$.

There will be no Z-point whenever $\ln Z(G) > F(G,0)$, or $r > 1$. In the case of stars this condition reads $\ln n > 2$, i.e., $n > e^2 = 7.389$. Hence, stars with 8 or more vertices have no Z-point, as noted before. Other trees without Z-point are also highly branched and, hence, are not molecular graphs.

Table 3. Asymptotic Behavior of Typical Series of Tree Graphs

Type	n	$n - n_0$ $= F(G,0)$	Z	$\lim_{n \to \infty} r$ $r = \ln Z / F(G,0)$	$\lim_{n \to \infty} x_H$ (estimated)
P_n	n	$2[n/2]$	$Z_n = \{\alpha^{n+1} - \beta^{n+1}\}/\sqrt{5}$ $\alpha = (1+\sqrt{5})/2 \quad \beta = (1-\sqrt{5})/2$ $= 1.6180 \qquad\qquad = -0.6180$	$\ln\{(1+\sqrt{5})/2\}$ $= 0.4812$	~ 1.22
E_k	$2k+2$	$2k$	$Z_k = \{\alpha^{\kappa+1} + \beta^{\kappa+1}\}/2$ $\alpha = 1+\sqrt{2} \quad \beta = 1-\sqrt{2}$ $= 2.4142 \qquad = -0.4142$	$\{\ln(1+\sqrt{2})\}/2$ $= 0.4407$	~ 1.18
J_k	$3k+1$	$2k$	$Z_k = \{\alpha^{\kappa+1} - \beta^{\kappa+1}\}/2\sqrt{3}$ $\alpha = 2+\sqrt{3} \quad \beta = 2-\sqrt{3}$ $= 3.7321 \qquad = 0.2679$	$\{\ln(2+\sqrt{3})\}/2$ $= 0.6585$	~ 1.14
C_k	$3k+2$	$2k$	$Z_k = \{(\sqrt{13}+2)\alpha^{\kappa} + (\sqrt{13}-2)\beta^{\kappa}\}/\sqrt{13}$ $\alpha = (3+\sqrt{13})/2 \quad \beta = (3-\sqrt{13})/2$ $= 3.3028 \qquad\quad = -0.3028$	$\{\ln(3+\sqrt{13})/2\}/2$ $= 0.5974$	~ 1.11
T_k	$4k+1$	$2k$	$Z_k = \{\alpha^{\kappa+1} - \beta^{\kappa+1}\}/\sqrt{21}$ $\alpha = (5+\sqrt{21})/2 \quad \beta = (5-\sqrt{21})/2$ $= 4.7913 \qquad\quad = 0.2087$	$\{\ln(5+\sqrt{21})/2\}/2$ $= 0.7834$	~ 0.995
S_n	n	2	$Z_n = n$	∞	—

The types of graphs are given in Fig. 2.

All Chemical Trees Have a *Z*-Point

We now show that the inequality $F(G,0) > \ln Z(G)$ is obeyed by all chemical trees. In order to accomplish this task we find a lower bound for $F(G,0)$ and an upper bound for $\ln Z(G)$, and then demonstrate that the lower bound for $F(G,0)$ is greater than the upper bound for $\ln Z(G)$.

A Lower Bound for $F(G, 0)$. For $x = 0$ the Coulson function is equal to[34,37] $n - n_0$, where n is the number of vertices of the graph G and n_0 is the number of zero eigenvalues[31] of G. Therefore, for fixed n, the graphs with maximum number of zero eigenvalues will have the smallest values of $F(G,0)$.

We thus have to find the chemical trees with a fixed number (n) of vertices and with maximum n_0. For the first few values of n, these trees are identified by direct checking (See Fig. 3). For $n = 9$ the respective tree T_2 (representing 2,2,4,4-tetramethyl-pentane) has vertices of degree 4, 2, and 1, and no vertex of degree 3. Further, the vertex of degree 2 is adjacent to the two vertices of degree 4.

The general construction proceeds as follows:

Step 0: Start with an n-vertex tree $X_n = T_k$ with $n = 4k+1$ ($k > 1$) possessing vertices of degree 1, 2, and 4, but no vertex of degree 3, such that each vertex of degree 2 is adjacent to two vertices of degree 4 and no two vertices of degree 4 are mutually adjacent. Such trees have maximum n_0 among all n-vertex chemical trees. This, for instance, may be T_k ($= X_n$) as depicted in Fig. 2.

Step 1: Construct a tree X_{n+1} by attaching a vertex of degree 1 to a vertex of degree 2 of X_n. This tree has maximum n_0 among all $(n+1)$-vertex chemical trees, and $n_0(X_{n+1}) = n_0(X_n) - 1$.

Step 2: Construct a tree X_{n+2} by attaching a vertex of degree 1 to the (unique) vertex of degree 3 of X_{n+1}. This tree has maximum n_0 among all $(n+2)$-vertex chemical trees, and $n_0(X_{n+2}) = n_0(X_n)$.

Step 3: Construct a tree X_{n+3} by inserting a vertex of degree

Fig. 3. The chemical tree graphs with the largest n_0 values among the isomers. The asterisked graphs for $n = 6$–8 have the minimum x_H values among their isomers. Observe the periodic increase of n_0 value with n as relevant to the strategy for designing the tree graph with the largest n_0 (See Fig. 4).

2 between two adjacent vertices of degree 4 of X_{n+2}. This tree has maximum n_0 among all $(n+3)$-vertex chemical trees, and $n_0(X_{n+3}) = n_0(X_n) + 1$.

Step 4: Construct a tree X_{n+4} by inserting a vertex of degree 2 between two adjacent vertices of degree 4 of X_{n+3}. This tree has maximum n_0 among all $(n+4)$-vertex chemical trees, and $n_0(X_{n+4}) = n_0(X_n) + 2$. Note that X_{n+4} is T_{k+1} and again a tree possessing the structural features required in Step 0. Therefore we may now repeat Step 1, etc.

The above described construction of chemical trees with maximum n_0 is illustrated in Fig. 4.

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Starting with $X_n = T_k$, $n = 4k+1$

$X_n = T_k$ X_{n+1} X_{n+2}

Δn_0 -1 $+1$

X_{n+3} $X_{n+4} = T_{k+1}$
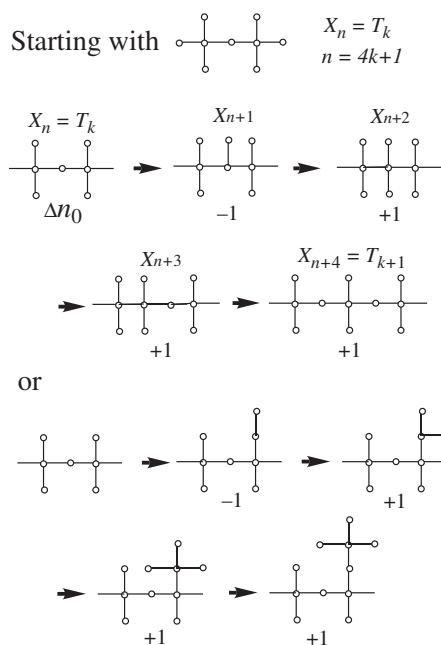
$+1$ $+1$

or

-1 $+1$

$+1$ $+1$

Fig. 4. Constructing chemical trees with maximum number of zero eigenvalues among isomers. For details see text.

In Fig. 4 is shown also an alternative construction of trees with maximum n_0.

The above described construction procedure leads directly to the following result:

$$(n_0)_{max} = \begin{cases} (n+1)/2 & \text{for} \quad n = 1, 5, 9, 13, 17, \cdots \\ (n-2)/2 & \text{for} \quad n = 2, 6, 10, 14, 18, \cdots \\ (n-1)/2 & \text{for} \quad n = 3, 7, 11, 15, 19, \cdots \\ n/2 & \text{for} \quad n = 4, 8, 12, 16, 20, \cdots. \end{cases} \quad (16)$$

Therefore, for any value of n,

$$(n_0)_{max} \leq (n+1)/2 \quad (17)$$

implying

$$F(G, 0) \geq (n-1)/2, \quad (18)$$

which is derived by using Eq. 13.

An Upper Bound for $\ln Z(G)$. Denote by P_n, the path graph, or the n-vertex path (See Fig. 2). It has been shown[1,9] that $Z(P_n)$ is just the n-th Fibonacci number. In view of this, using a well known formula for Fibonacci numbers,

$$Z(P_n) = \frac{1}{\sqrt{5}} \left[\left(\frac{1+\sqrt{5}}{2} \right)^{n+1} - \left(\frac{1-\sqrt{5}}{2} \right)^{n+1} \right] \quad (19)$$

from which it follows

$$Z(P_n) \leq \frac{1}{\sqrt{5}} \left[\left(\frac{1+\sqrt{5}}{2} \right)^{n+1} + \left(\frac{1-\sqrt{5}}{2} \right)^{n+1} \right]$$

$$= \left(\frac{1+\sqrt{5}}{2} \right)^n \left(\frac{1+\sqrt{5}}{2\sqrt{5}} \right) (1 + g_n)$$

where

$$g_n = \left(\frac{\sqrt{5}-1}{\sqrt{5}+1} \right)^{n+1} = 0.3820^{n+1}.$$

For $n = 9$ the term g_n is equal to 0.0000252, and for larger n one can safely use the approximation $\ln(1 + g_n) \approx g_n$, and then

$$\ln Z(P_n) \leq n \ln \frac{1+\sqrt{5}}{2} + \ln \frac{1+\sqrt{5}}{2\sqrt{5}} + g_n. \quad (20)$$

Further, for $n \geq 10$ the term g_n is several orders of magnitude smaller than the other two terms occurring on the right-hand side of Eq. 20 and may be neglected, resulting in the inequality

$$\ln Z(P_n) \leq 0.4812n - 0.3235.$$

It has been shown[11] that $Z(P_n)$ is greater than the topological index Z of any other n-vertex tree. Bearing this in mind, we conclude that the logarithm of the topological index Z of any n-vertex tree is bounded from above as follows,

$$\ln Z(G) \leq 0.4812n - 0.3235 \quad (21)$$

which is just the required upper bound.

Completion of the Proof. The fact that all chemical trees with 9 or fewer vertices have a Z-point can easily be verified by direct checking. (In fact, we have verified this fact for all trees with 20 or fewer vertices as seen in Table 1.)

If the inequality

$$(n-1)/2 > 0.4812n - 0.3235 \quad (22)$$

is satisfied, then in view of the relations 18 and 21, the inequality $F(G, 0) > \ln Z(G)$, or $r < 1$, will hold, implying the existence of the Z-point of the graph G. Now, inequality 22 is readily solved, yielding $n > 9.388$. Consequently, all chemical trees with 10 or more vertices have a Z-point. Then all chemical trees have a Z-point.

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