match no. 14 pp. 213-233 1983

# THE SMALLEST GRAPHS, TREES, AND 4-TREES WITH DEGENERATE TOPOLOGICAL INDEX J

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(Received: February 1983)

Abstract

The degeneracy, i.e., equal values for non-isomorphic graphs, of the topological index J is explored systematically. J-equivalent non-isomorphic graphs have at least six points, in which case these graphs are tri- or tetra-cyclic; for mono- or bi-cyclic J-equivalent graphs, the smallest order is eight. The unique smallest order pair of trees having the same J-value (and the same distance sum sequence) consists of trees with ten points. There are six pair of smallest order J-equivalent 4-trees. These are realized as 4-trees on twelve points. Theorems are presented for constructing these graphs and other J-equivalent graphs of higher orders. A comparison with Randić's molecular connectivity shows that J has lower degeneracy.

## 1A. Chemical Introduction

Topological indices (reviews [1 - 3]) are used to convert the structure of a molecule (symbolized by a graph) into a numerical value. This value can then be used for correlating this molecular structure with its chemical, physical, or biological properties. Such an approach is particularly useful in drug design [1 - 3].

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*Supported in part by a grant from the Pace University Scholarly Research Committee.

The current best and most used topological index, the molecular connectivity $\chi$, was proposed by Randić [4] and is based on point degrees (see graph-theoretical definitions below).

A general problem of topological indices is that the structure of a molecule cannot be retrieved from the topological index, i.e., the conversion of structure to topological index works only in one direction. One of the reasons is that topological indices are degenerate, i.e., two or more non-isomorphic structures may lead to the same value for a given topological index.

A new, highly discriminating topological index, denoted by J, was recently described [5, 6]. Since the discriminating ability of an index is inversly related to its degeneracy, we present here a systematic exploration of the degeneracy of J. A comparision with Randić's molecular connectivity shows that J has lower degeneracy.

## 1B. Graph-Theoretical Introduction

Let G denote a connected graph with q lines, n points, and cyclomatic number $\mu = q - n + 1$; E(G) the line set of G and $s_a$ the sum of the distances from the point a to all other points of G. We call $s_a$ the distance sum at a. Then,

$$J(G) = \frac{q}{\mu + 1} \sum_{E(G)} \frac{1}{\sqrt{s_a s_b}}$$

where $\{a,b\} \in E(G)$, is called the J-Index of G.

If J(G) = J(H), then the graphs G and H are said to be J-equivalent.

We are interested in determining how effective the J-Index is in distinguishing between graphs.

The order of a graph is its number of points. The number of lines incident to a point is called the degree of that point. If each point of a graph has the same degree r, the graph is called r-regular.

A tree is called a 4-tree if it does not have any points of degree greater than 4. We have found that 12 is the least order for which there exists a pair of J-equivalent non-isomorphic 4-trees (see Section 4).

In passing we note that if there are no restrictions on the class of graphs being considered, then 6 is the least order realizable by a pair of J-equivalent non-isomorphic graphs (see Section 2). However, graphs of chemical interest are those with specified constraints and in particular those with bounded degree. Thus, investigations of the type considered here are always carried on within a given class of graphs.

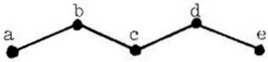
Included in what follows are descriptions of some general methods for constructing J-equivalent graphs (see Section 3).

## 2. Observations and Examples

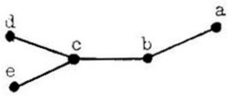
If G has point set $\{v_1,v_2,\ldots,v_n\}$ and $d_{ij}$ is the number of points in G at distance j from $v_i$, then the sequence $(d_{i0},d_{i1},d_{i2},\ldots,d_{ij},\ldots)$ is called the distance degree sequence of $v_i$ in G. Note that $d_{i0} = 1$ and $d_{i1} = \deg v_i$, the degree of $v_i$. The n-tuple of distance degree sequences arranged in lexicographic order is the distance degree sequence of G. These sequences are denoted DDS($v_i$) and DDS(G) respectively.

Note 1. We use { } to denote sets, i.e., unordered collections of distinct objects, and [ ] to denote multi-sets, i.e., unordered collections of objects in which repetitions are allowed (see [7; p. 60]). Ordered collections of objects in which repetitions are allowed are called sequences and are denoted by using ( ). If an entry s is repeated t times in a sequence, the subsequence s,s,...,s (t terms) is replaced by $s^t$.

As an illustration of these concepts consider the three isomeric pentanes:




$\mathbf{1}$

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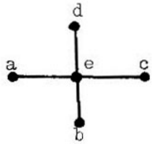



$\mathbf{3}$

For $\mathbf{1}$ we have: DDS(a) = DDS(e) = (1,1,1,1,1)
DDS(b) = DDS(d) = (1,2,1,1)
DDS(c) = (1,2,2)
and DDS($\mathbf{1}$) = $((1,1,1,1,1)^2,(1,2,1,1)^2,(1,2,2))$.

Graph $\mathbf{2}$ yields: DDS(a) = (1,1,1,2), DDS(b) = (1,2,2), DDS(c) = (1,3,1)
DDS(d) = DDS(e) = (1,1,2,1)
and DDS($\mathbf{2}$) = $((1,1,1,2),(1,1,2,1)^2,(1,2,2),(1,3,1))$.

The sequences for $\mathbf{3}$ are: DDS(a) = DDS(b) = DDS(c) = DDS(d) = (1,1,3)
DDS(e) = (1,4)
and DDS($\mathbf{3}$) = $((1,1,3)^4,(1,4))$.

The <u>distance sum sequence of G</u>, which we denote by D(G), is the sequence of distance sums of the points of G arranged in increasing magnitude.

The distance sum sequences of $\mathbf{1}$, $\mathbf{2}$, and $\mathbf{3}$ are: D($\mathbf{1}$) = $(6,7^2,10^2)$ D($\mathbf{2}$) = $(5,6,8,9^2)$ and D($\mathbf{3}$) = $(4,7^4)$.

<u>Theorem 1</u>. If G and H are connected graphs having the same distance degree sequence and $e \longrightarrow \theta(e)$ is a one-to-one function of E(G) onto E(H) such that

$$[DDS(a),DDS(b)] = [DDS(u),DDS(v)]$$

for each $e = \{a,b\}$ and $\theta(e) = \{u,v\}$, then G and H are J-equivalent.

Proof. First, if DDS(G) = DDS(H), then G and H have the same number of points n, the same number of lines q, and consequently the same cyclomatic number $\mu$. Thus, $q/(\mu + 1)$ is the same for G and H.

Second, if a point x has distance degree sequence $(1, d_{x1}, d_{x2}, \dots, d_{xj}, \dots)$, then it has distance sum $s_x = \sum_j j d_{xj}$. Thus, not only do G and H have the same distance sum sequence, but because $\theta$ is a one-to-one correspondence from E(G) to E(H) preserving the associated pairs of distance degree sequences for each line, $\theta$ induces a one-to-one correspondence between the two multi-sets of products $[\dots, s_a s_b, \dots]$ and $[\dots, s_u s_v, \dots]$ where $\theta(\{a,b\}) = \{u,v\}$.

By definition

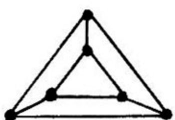
$$J(G) = \frac{|E(G)|}{\mu(G) + 1} \sum_{E(G)} \frac{1}{\sqrt{s_a s_b}} \qquad \text{and } J(H) = \frac{|E(H)|}{\mu(H) + 1} \sum_{E(H)} \frac{1}{\sqrt{s_u s_v}} .$$

We have already noted that $|E(G)|/(\mu(G) + 1) = |E(H)|/(\mu(H) + 1)$. From the observations of the preceding paragraph we have

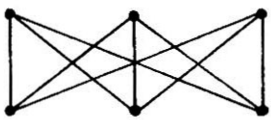
$$\sum_{E(G)} (\sqrt{s_a s_b})^{-1} = \sum_{E(H)} (\sqrt{s_u s_v})^{-1}.$$

Therefore, G and H are J-equivalent.[]

Note 2. Since the graphs $\underset{\approx}{4}$ and $\underset{\approx}{5}$ shown below each have 6 points, 9 lines, and the same distance degree sequence at each point, namely, (1,3,2), the conditions of Theorem 1 are trivially satisfied. Thus, $\underset{\approx}{4}$ and $\underset{\approx}{5}$ are J-equivalent and because there are no J-equivalent pairs of graphs on 5 or less points, we have that 6 is the least order for which a pair of non-isomorphic graphs can be J-equivalent.

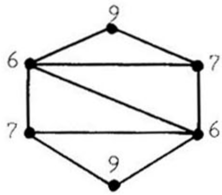


$\underset{\approx}{4}$



$\underset{\approx}{5}$

Graph 5 is the non-planar Kuratowski graph $K_{3,3}$ and the graphs 4 and 5 are 3-regular graphs with $\mu = 4$ (tetra-cyclic). Two other pairs of J-equivalent tetra-cyclic (non-regular) graphs on 6 points are shown below (see 6 and 7, 8 and 9). The points of the graphs are labelled by the distance sum at the point.

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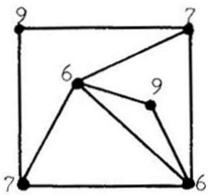


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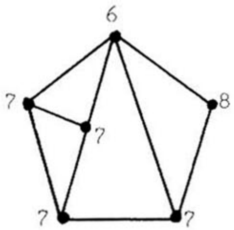


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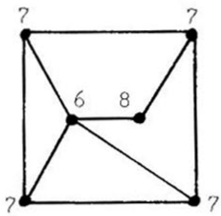


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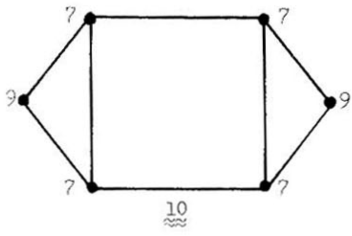
For the pair of smallest order J-equivalent tri-cyclic ($\mu = 3$) graphs we exhibit the two 6-point graphs 10 and 11.

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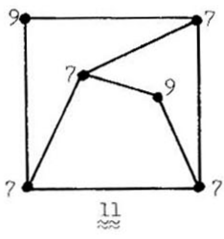


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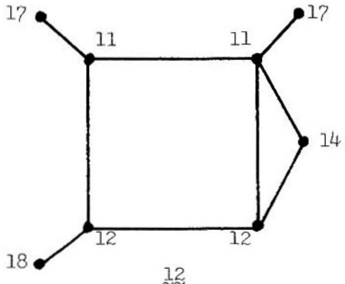
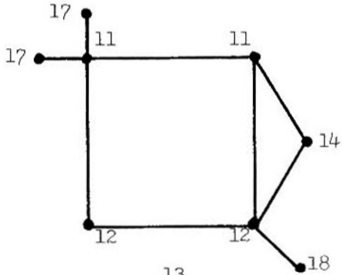
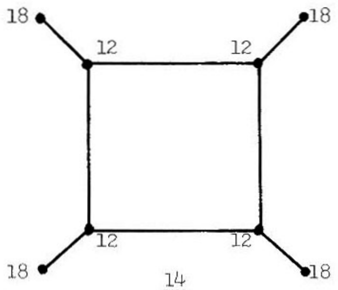
The smallest order pairs of bi-cyclic and mono-cyclic ($\mu = 2$ and $\mu = 1$, respectively) J-equivalent graphs have 8 points. There is one pair of each type (see **12** and **13**, **14** and **15**).




**12**




**13**

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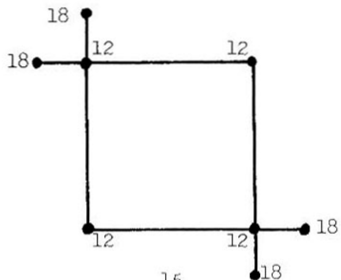



**15**

A graph is called *distance degree regular* (DDR) if each point in the graph has the same distance degree sequence (see [8]).

*Corollary 1a*. If G and H are connected DDR graphs having the same distance degree sequence, then G and H are J-equivalent.

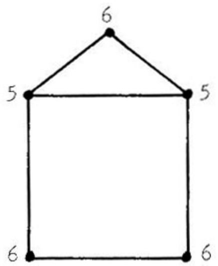
Proof. Since G and H have the same number of lines and the distance degree sequence is constant and equal for all points in both graphs any one-to-one function of E(G) onto E(H) is of the form θ. Thus, by Theorem 1, G and H are J-equivalent.□

Note 3. Same distance degree sequence (which implies same distance sum sequence) does not imply same J-Index. E.g., the following graphs **16** and **17** have the same distance degree sequence. Namely, DDS(**16**) = DDS(**17**) = $((1,3,1)^2,(1,2,2)^3)$. However, these graphs are not J-equivalent.

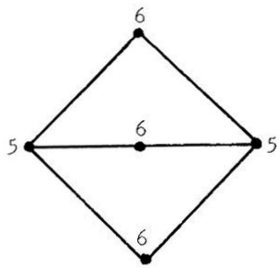
$$J(\mathbf{16}) = \frac{6}{3}\left(\frac{4}{\sqrt{30}} + \frac{1}{5} + \frac{1}{6}\right) = 2.1939$$

$$J(\mathbf{17}) = \frac{6}{3}\left(\frac{6}{\sqrt{30}}\right) = 2\left(\frac{6}{\sqrt{30}}\right) = 2.1909 \quad \text{(see [5; Figure 1] and [6])}$$

This example simultaneously illustrates that 5 is the smallest order for which there exists a pair of connected non-isomorphic graphs having the same distance degree sequence or the same distance sum sequence (see [9]).




**16**




**17**

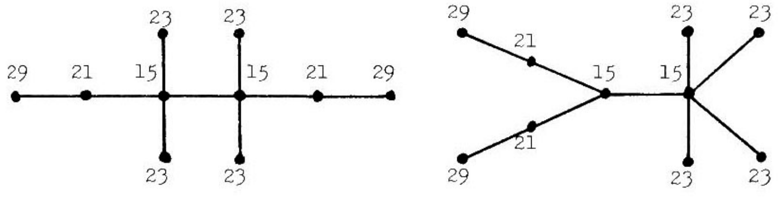
Corollary 1b. All r-regular, diameter 2, graphs of order n are J-equivalent.

Proof. The distance degree sequence of an r-regular, diameter 2, graph of order n is $((1,r,n-r-1)^n)$. Thus, every such graph is DDR with the same DDS. By Corollary 1a, all such graphs are J-equivalent.[]

Corollary 1c. The complements of all r-regular graphs of order n having diameter $\geq 3$ are J-equivalent.

Proof. The complement of an r-regular graph of diameter $\geq 3$ is an $(n-r-1)$-regular graph of order n having diameter 2 (see [10; Theorem 2, p. 2]). Thus, by Corollary 1b, all such graphs are J-equivalent.[]

Note 4. Same distance sum sequence does not imply same distance degree sequence. E.g., the graphs 18 and 19 shown below have the same distance sum sequence. As was noted by Z. Miller ([11; p. 316] and [12]) these form the unique smallest order pair of trees having the same distance sum sequence. However, 19 has a point of degree 5 whereas 18 does not, consequently, DDS(18) $\neq$ DDS(19).

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Corollary 1d. If G and H are connected graphs having the same distance sum sequence and $e \longrightarrow \theta(e)$ is a one-to-one function of $E(G)$ onto $E(H)$ such that

$$[s_a, s_b] = [s_u, s_v]$$

for each $e = \{a,b\}$ and $\theta(e) = \{u,v\}$, then G and H are J-equivalent.

Proof. See the proof of Theorem 1. If hypothesis is satisfied, then G and H have the same number of points n, the same number of lines q, and consequently the same $q/(\mu + 1)$ value. Furthermore, $\theta$ induces a one-to-one correspondence between $[\ldots, s_a s_b, \ldots]$ and $[\ldots, s_u s_v, \ldots]$. Thus, $J(G) = J(H)$.[]

Note 5. Applying Corollary 1d we observe that the trees of Note 4 are J-equivalent. Furthermore, by checking all trees of order $\leq 9$, it is found that these 10-point trees form the unique pair of smallest order J-equivalent trees.

## 3. Some Construction Methods

There are methods for constructing pairs of non-isomorphic graphs having the

(i) same distance degree sequence

or

(ii) same distance sum sequence.

Such pairs of graphs are good candidates for having the same J-Index.

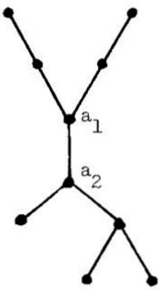
Although (i) implies (ii), the two construction methods, which are described below (see Theorems 2 and 3), yield different types of graphs. Thus, both methods should be considered if one is interested in finding J-equivalent graphs.

Theorems 2 and 3 are obtained from P. J. Slater [11].

Theorem 2. Let A be a graph such that points $a_1$ and $a_2$ in A have the same distance degree sequence. Let $b_1$ be a point in a graph $B_1$ and $b_2$ a point in a graph $B_2$ such that $b_1$ and $b_2$ have the same distance degree sequence in $B_1$ and $B_2$ respectively.

If G is the graph constructed from A, $B_1$, and $B_2$ by identifying $a_1$ with $b_1$ and identifying $a_2$ with $b_2$ and H is the graph constructed from A, $B_1$, and $B_2$ by identifying $a_1$ with $b_2$ and identifying $a_2$ with $b_1$, then G and H have the same distance degree sequence and consequently the same distance sum sequence.

Note 6. As an application of Theorem 2 consider the following graphs:

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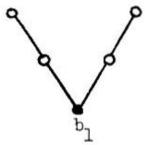


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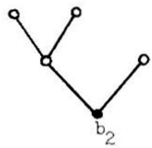


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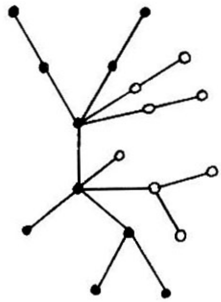
Since $DDS(a_1) = DDS(a_2) = (1,3,4,2)$ and $DDS(b_1) = DDS(b_2) = (1,2,2)$ we can construct graphs 23 and 24 as instructed in Theorem 2. The open points clearly indicate the locations of graphs 21 and 22. Thes graphs, originally constructed by P. J. Slater [12], have the same distance degree sequence. In addition, they determine 18 to be the smallest order example found to date of a pair of non-isomorphic trees having the same distance degree sequence.



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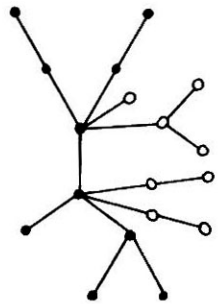

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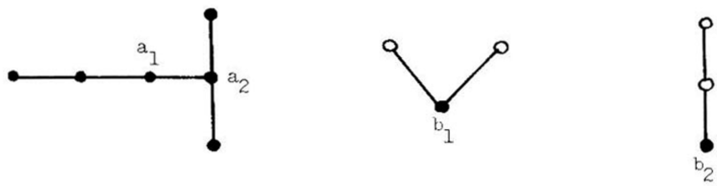
Theorem 3. Let A be a graph such that points $a_1$ and $a_2$ in A have the same distance sum. Let $b_1$ be a point in a graph $B_1$, $b_2$ a point in a graph $B_2$, and such that $B_1$ and $B_2$ have the same number of points.

If G is the graph constructed from A, $B_1$, and $B_2$ by identifying $a_1$ with $b_1$ and identifying $a_2$ with $b_2$, and H is the graph constructed from A, $B_1$, and $B_2$ by identifying $a_1$ with $b_2$ and identifying $a_2$ with $b_1$, then G and H have the same distance sum sequence.

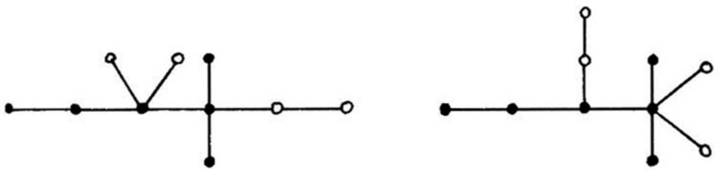
Note 7. If in Theorems 2 and 3, the points $a_1$ and $a_2$ are non-equivalent and the graphs $(B_1, b_1)$ and $(B_2, b_2)$ are non-isomorphic as rooted graphs, then G and H are non-isomorphic.

Note 8. Since same distance degree sequence implies same distance sum (see proof of Theorem 1) the graphs 20 through 24 also provide an illustration of Theorem 3. However, a sharper illustration is obtained if one uses the graphs:




25 26 27

Since $D(a_1) = D(a_2) = 8$, we can use Theorem 3 to construct graphs 28 and 29.



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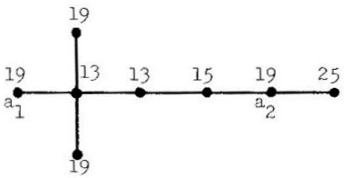
These graphs are precisely graphs 18 and 19 of Section 2 and, as noted there, the unique smallest pair of trees having the same distance sum sequence.

4. Least Order Pairs of J-Equivalent Non-Isomorphic 4-Trees

We have determined by calculation of the J-Index that there are no J-equivalent pairs of 4-trees on $\leq$ 11 points.

By applying Theorem 3 we have obtained six pairs of 4-trees which pairwise have the same distance sum sequence. Then, noting that a function $\theta$ of the type required in Corollary 1d is readily obtained for each of these pairs, it follows that these trees are pairwise J-equivalent. That there are no other minimal order J-equivalent 4-trees was confirmed by calculation of the J-Index of all 4-trees with up to 11 points (no degeneracy found) and of the 355 4-trees on 12 points (six degenerate pairs found).

Starting with the six 4-trees 30 through 35, we use Theorem 3, Corollary 1d, and graphs 26 and 27 to obtain the above mentioned six pairs of J-equivalent 4-trees on 12 points (see 36 through 47).

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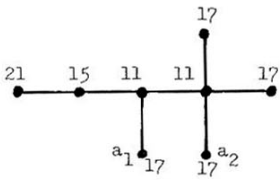


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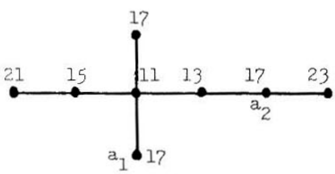


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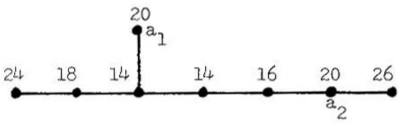


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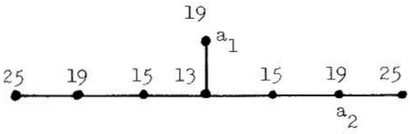


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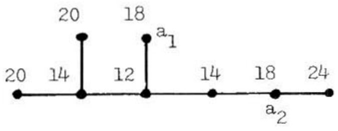


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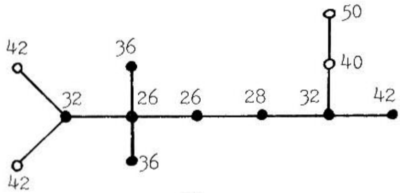


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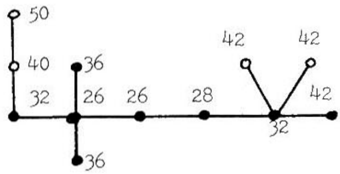


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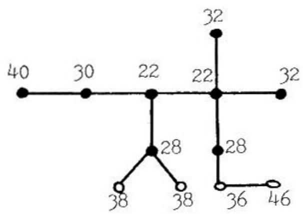
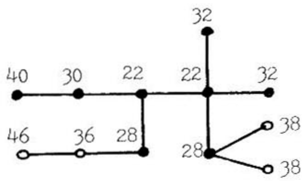



38

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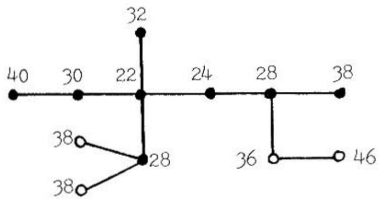


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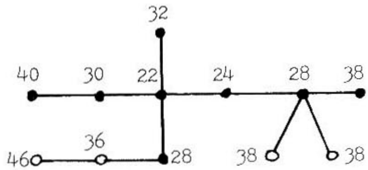


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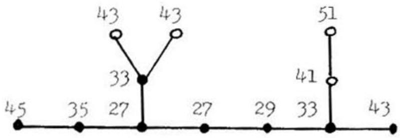


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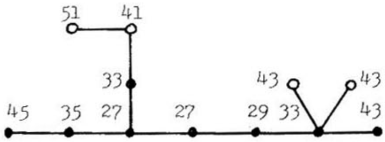


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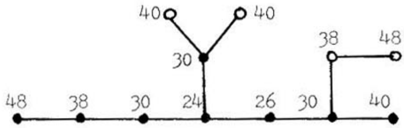
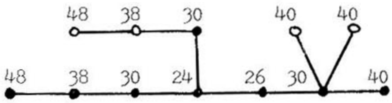
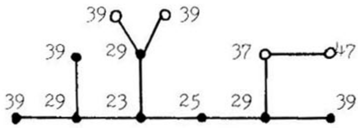


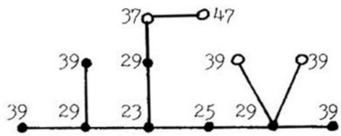

44




45

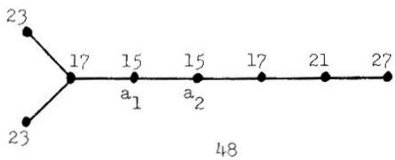



46



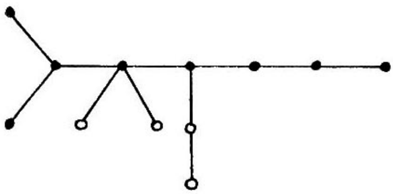

47

Note 9. The trees constructed above are not arrived at uniquely. For example, using the same method, trees 38 and 39 can be derived from 48, 26, and 27 or from 25, 49, and 50.

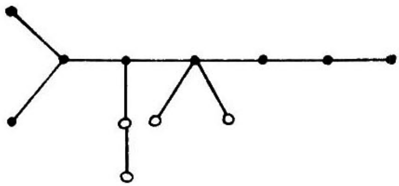



48

**48** combined with **26** and **27** yields:

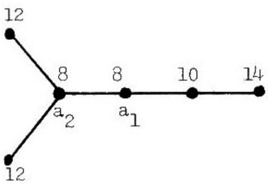


**39**

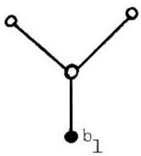


**38**

Combining **25**, **49**, and **50** also yields **38** and **39**.

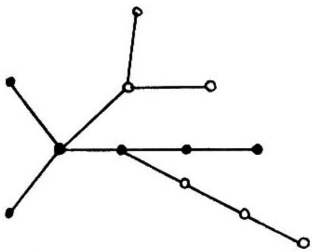



**25**

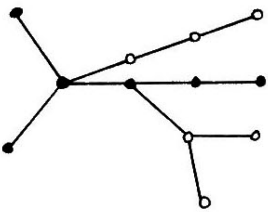



**49**


**50**



**39**



**38**

5. Comparision with Randić's Molecular Connectivity

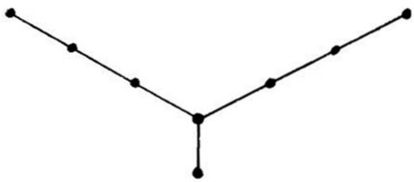
The topological index $\chi$, introduced by M. Randić [3,4] and called the molecular connectivity, had the lowest degeneracy among all previous single topological indices [13]. This index $\chi$ is based on point degrees deg a, deg b of adjacent vertices a, b, and is defined

$$\chi(G) = \sum_{E(G)} \frac{1}{\sqrt{(\deg a)(\deg b)}}$$

where $\{a,b\} \in E(G)$.

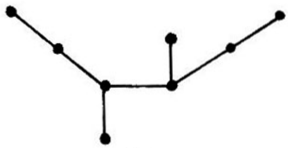
In order to make comparisions with J, we recall from the literature [4,13] or we determine for the purpose of this paper the following:

The smallest order $\chi$-equivalent trees have 8 points (see 51 and 52, 53 and 54). There are just two such pairs among the 23 trees of order 8 and as can be seen these are 4-trees.

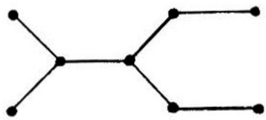


51

52

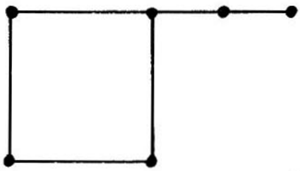


53

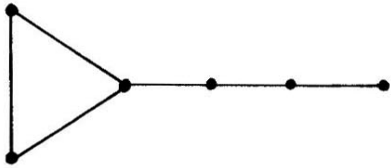


54

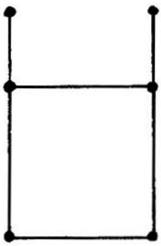
Among the 29 mono- or bi-cyclic graphs on 6 points and degree no greater than 4, there exist two pairs of $\chi$-equivalent mono-cyclic graphs and three $\chi$-equivalent bi-cyclic graphs (see 55 and 56, 57 and 58; 59, 60, and 61).



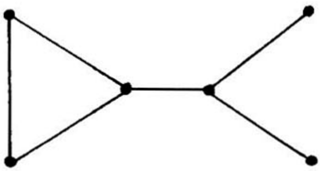
55



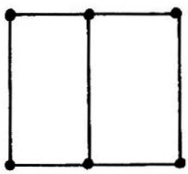
56



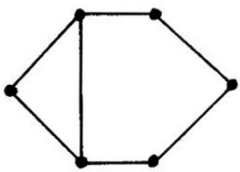
57



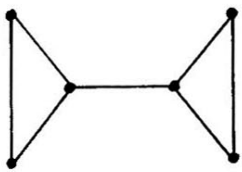
58



59



60



61

By way of comparison, J starts to become degenerate for trees of order 10 (one pair out of 106 such trees), for 4-trees of order 12 (six pairs out of 355 4-trees), and for mono- or bi-cyclic graphs of order 8 (two pairs out of 250 such graphs).

Clearly, J is much less discriminating than $\chi$. It should be recalled that, according to a comparison between all previously defined topological indices [13], Randić's index $\chi$ was among those with the lowest degeneracy.

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