Trees with Extremal Hyper-Wiener Index: Mathematical Basis and Chemical Applications

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Trees with minimal and maximal hyper-Wiener indices (WW) are determined: Among n-vertex trees, minimum and maximum WW is achieved for the star-graph (S_n) and the path-graph (P_n), respectively. Since $WW(S_n)$ is a quadratic polynomial in n,, whereas $WW(P_n)$ is a quartic polynomial in n, the hyper-Wiener indices of all n-vertex trees assume values from a relatively narrow interval. Consequently, the hyper-Wiener index must have a very low isomer-discriminating power. This conclusion is corroborated by finding large families of trees, all members of which have equal WW-values.

INTRODUCTION

The hyper-Wiener index (WW) is a graph invariant, put forward by Randić a few years ago[1] as a kind of extension of the classical Wiener-index-concept. Randić's article[1] stimulated a large number of subsequent researches[2−10] on WW, and the main properties of this topological index are nowadays relatively well understood.

Randić's starting point was the following long-known[11,12] property of the Wiener index (W) of trees. Let T be a tree (i.e., a connected and acyclic graph). Let e be an edge of T, joining the (adjacent) vertices u and v. Denote by $n_u(e)$ the number of vertices of T lying on one side of the edge e, closer to vertex u. Denote by $n_v(e)$ the number of vertices of T lying on the other side of the edge e, closer to vertex v. (Because T is acyclic, the quantities $n_u(e)$ and $n_v(e)$ are unambiguously determined for every edge.) Then the Wiener index of T satisfies the relation[11]

$$W(T) = \sum_e n_u(e) n_v(e)$$

in which the summation goes over all edges of T.

Now, instead of adjacent vertices, Randić extended the consideration to arbitrary pairs of vertices u,v of the tree T. These vertices are joined by a unique path which we denote by p. Denote by $n_u(p)$ the number of vertices of T lying on one side of the path p, closer to vertex u. Denote by $n_v(p)$ the number of vertices of T lying on the other side of the path p, closer to vertex v. (Again, because T is acyclic, the quantities $n_u(p)$ and $n_v(p)$ are unambiguously determined for every path.) Then the hyper-Wiener index of T is defined by means of the relation[1]

$$WW(T) = \sum_p n_u(p) n_v(p) \tag{1}$$

in which the summation goes over all paths of T.

As well known, the Wiener index is defined as the sum of distances between all pairs of vertices of the respective graph:

$$W(G) = \sum_{x<y} d(x,y|G)$$

whereby $d(x,y|G)$ we denote the distance of vertices x and y in the graph G. (Recall that $d(x,y|G)$ is equal to the number of edges in a shortest path, joining x and y.) A nice and comprehensive review of the Wiener index is in Ref. 13.

It has been demonstrated[6] that in the case of trees the following noteworthy identity is satisfied:

$$WW(T) = \frac{1}{2}[\sum_{x<y} d(x,y|T)^2 + \sum_{x<y} d(x,y|T)] \tag{2}$$

The original Randić definition[1] of the hyper-Wiener index, namely eq 1, is not applicable to cycle-containing graphs. In view of this, the right-hand side of formula 2 is extended to all graphs, serving as a suitable general definition[6,8−10] of the hyper-Wiener index. Thus, if G is an arbitrary connected graph, then its hyper-Wiener index is given by

$$WW(G) = \frac{1}{2}[\sum_{x<y} d(x,y|G)^2 + \sum_{x<y} d(x,y|G)] \tag{3}$$

THE MAIN RESULTS

Let, as usual, S_n and P_n denote the n-vertex star-graph and path-graph, respectively. [As an example, in Figure 1 are depicted the 9-vertex star- and the path-graphs.]

It is known for some time[14,15] that S_n and P_n are extremal with regard to the Wiener index. Entringer et al.[14] were first to formulate the following result. Note, however, that results equivalent to Theorem 1 were stated already by Bonchev and Trinajstić[15] but not in a theorematic form.

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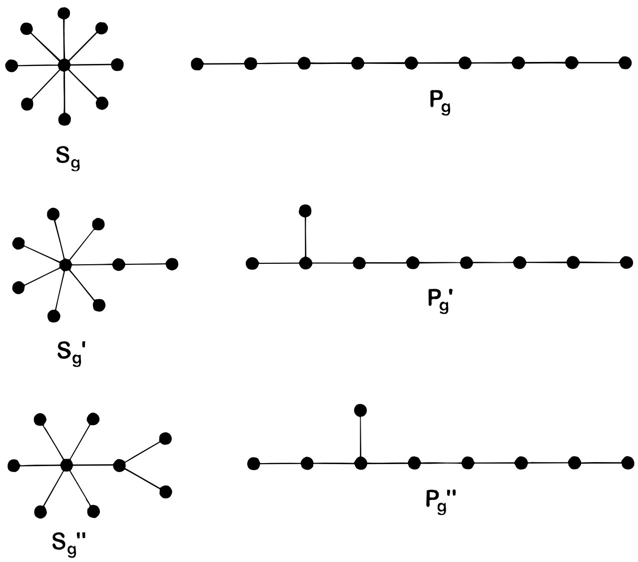

Figure 1. *n*-vertex trees with minimal and maximal hyper-Wiener index, shown for the case of $n = 9$.

Theorem 1. (a) If T is an n-vertex tree, then for all values of n, $n \geq 1$,

$$W(S_n) \leq W(T) \leq W(P_n)$$

(b) If, in addition, T differs from S_n and P_n, then for all values of n, $n \geq 5$,

$$W(S_n) < W(T) < W(P_n)$$

Recall that for $n \leq 4$ there are no n-vertex trees different from S_n and P_n.

We now demonstrate that a fully analogous regularity applies also for the hyper-Wiener index.

Theorem 2. (a) If T is an n-vertex tree, then for all values of n, $n \geq 1$,

$$WW(S_n) \leq WW(T) \leq WW(P_n)$$

(b) If, in addition, T differs from S_n and P_n, then for all values of n, $n \geq 5$,

$$WW(S_n) < WW(T) < WW(P_n)$$

PROOF OF THEOREM 2

We first notice that Theorem 2 consists of two statements: (1) that the star-graph has minimal *WW* and (2) that the path-graph has maximal *WW*. These will be proved separately.

In order to deduce Theorem 2 we establish two somewhat stronger results.

First Auxiliary Inequality. Let G be an arbitrary connected graph, possessing n vertices and m edges, and let its hyper-Wiener index be defined via eq 3. Then the number of pairs of distinct vertices of G is equal to $n(n-1)/2$.

Exactly m pairs of vertices of G are at distance one. The remaining $n(n-1)/2-m$ pairs of vertices are at distances which are two or greater than two. Therefore,

$$\sum_{x<y} d(x,y|G) \geq m \times 1 + [n(n-1)/2 - m] \times 2$$

$$\sum_{x<y} d(x,y|G)^2 \geq m \times 1^2 + [n(n-1)/2 - m] \times 2$$

which substituted back into eq 3 yields

$$WW(G) \geq \frac{3}{2}n(n-1) - 2m \tag{4}$$

Equation 4 is a general lower bound for the hyper-Wiener index. For trees $m = n - 1$, and the inequality 4 becomes

$$WW(T) \geq \frac{1}{2}(n-1)(3n-4) \tag{5}$$

Now, in the star-graph all distances are either one or two. Therefore,

$$WW(S_n) = \frac{1}{2}(n-1)(3n-4) \tag{6}$$

and formula 5 can be rewritten as

$$WW(T) \geq \mathrm{WW}(S_n)$$

In any tree different from S_n there is at least one pair of vertices at distance greater than two. Consequently, $WW(S_n)$ is strictly less than $WW(T)$ whenever $T \neq S_n$.

This proves part (1) of Theorem 2.

Second Auxiliary Inequality. Let G be an arbitrary (connected) graph and r its arbitrary vertex. It is required that G possesses at least one more vertex in addition to r, i.e., that the subgraph G-r is not empty. Let a and b be two integers, such that $0 \leq a < b$.

Construct the graph H by attaching to the vertex r of G the terminal vertices of a path graph P_{a+1} and of another path graph P_b. The other terminal vertex of P_{a+1} is denoted by x (see Figure 2).

Construct the graph H' by attaching to the vertex r of G the terminal vertices of a path graph P_a and of another path graph P_{b+1}. This time by x we denote the other terminal vertex of P_{b+1} (see Figure 2).

It is seen that H' is obtained from H (and vice versa) by moving the vertex x from one position to the other. All structural details of the graphs H and H', except the position of the vertex x, are identical.

Consider the difference $WW(H') - WW(H)$. All distances in H and H', except those involving the vertex x, are equal and cancel out from the difference. The distances between the vertex x and the vertices in the two branches attached to vertex r (including the vertex r itself) are also equal and need not be considered. What remains are the distances between vertex x and the vertices of the subgraph G-r (see Figure 2). Therefore,

$$\begin{aligned} WW(H') - WW(H) = \frac{1}{2}\Big[\sum_y d(x,y|H')^2 + \sum_y d(x,y|H')\Big] - \\ \frac{1}{2}\Big[\sum_y d(x,y|H)^2 + \sum_y d(x,y|H)\Big] \end{aligned} \tag{7}$$

where all summations go over the vertices y , belonging to the subgraph G-r. For such vertices it is, evidently,

$$d(x,y|\mathrm{H}') = d(r,y|G) + b + 1 \tag{8}$$

$$d(x,y|\mathrm{H}) = d(r,y|G) + a + 1 \tag{9}$$

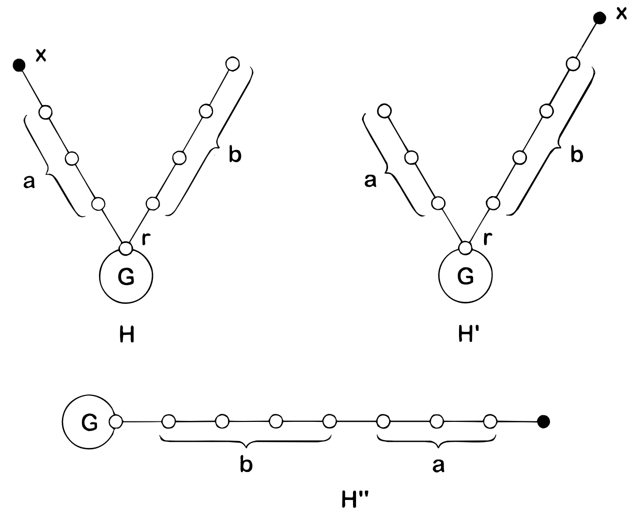

Figure 2. Graphs used in the proof of Theorem 2; if $a \leq$ b then $WW(H) < WW(H') < WW(H'')$.

When relations 8 and 9 are substituted back into eq 7 we obtain after some calculation

$$WW(H') - WW(H) = \frac{1}{2}(b-a)\sum_{y}[2d(r,y|G) + a + b + 3] \tag{10}$$

Every summand in the summation on the right-hand side of eq 10 is positive. Therefore the entire sum is also positive. Since the parameter b has be chosen to be greater than a, also the term $(b-a)$, occurring on the right-hand side of eq 10, is positive.

We thus arrive at our second auxiliary inequality:

$$WW(H') > WW(H) \tag{11}$$

Formula 11 means that if vertices are moved from a shorter branch to a longer branch (attached to the same vertex), then the hyper-Wiener index will necessarily increase. Repeating the construction $H \rightarrow H'$ a sufficient number of times we conclude that WW will achieve its maximum value when the shorter branch is completely removed. (This is graph H'' in Figure 2.)

Applying this argument to all branching points of an n-vertex tree we immediately conclude that the path-graph P_n (which has no branching points at all) has maximal hyper-Wiener index. Because all trees except the path-graph have at least one branching point, we also see that any n-vertex tree different from P_n has hyper-Wiener index strictly smaller than $WW(P_n)$.

This proves part (2) of Theorem 2.

MORE EXTREMAL TREES

Using the same arguments we may determine other trees with extremal value of the hyper-Wiener index. Without proof we state the following theorem. Let S_n', S_n'', P_n', and P_n'' be trees the structure of which is evident from the examples depicted in Figure 1.

Theorem 3. If T is an n-vertex tree which does not belong to the set $\{S_n, S_n', S_n'', P_n, P_n', P_n''\}$, then

$$WW(S_n) < WW(S_n') < WW(S_n'') < WW(T) < WW(P_n) < WW(P_n') < WW(P_n'')$$

Table 1. Size (i_n) of the Interval Containing the Hyper-Wiener Indices of All n-Vertex Trees, the Number of n-Vertex Trees (t_n), a Lower Bound (f_n), and the Exact Value (F_n) for the Average Size of Families of n-Vertex Trees with Equal Hyper-Wiener Indices (If $t_n > i_n$ Then $f_n = t_n/i_n$, Otherwise $f_n = 1$)

n	i_n	t_n	f_n	F_n
1	1	1	1	1
2	1	1	1	1
3	1	1	1	1
4	4	2	1	1
5	14	3	1	1
6	36	6	1	1
7	76	11	1	1
8	141	23	1	1
9	239	47	1	1.09
10	379	106	1	1.16
11	571	235	1	1.39
12	826	551	1	1.78
13	1156	1301	1.13	2.36
14	1574	3159	2.01	3.68
15	2094	7741	3.70	6.29
16	2731	19320	7.07	11.30
17	3501	48629	13.89	21.48
18	4421	123967	28.02	40.76
19	5509	317955	57.72	81.46
20	6784	823065	121.32	166.24
21	8266	2144505	259.44	334.97
22	9976	5623756	563.73	744.28
23	11936	14828074	1242.30	1591.85
24	14169	39299897	2773.65	
25	16699	104636890	6266.06	
26	19551	279793450	14310.95	

Trees to which Theorem 3 applies exist for $n \geq 7$.

ON THE ISOMER-DISCRIMINATING POWER OF THE HYPER-WIENER INDEX

The analytical expressions for the hyper-Wiener indices of star-graphs and path-graphs were previously deduced.[5] They are given by eqs 6 and 12:[16,17]

$$WW(P_n) = \frac{1}{24}n(n-1)(n+1)(n+2) = \binom{n+2}{4} \tag{12}$$

Equations 6 and 12 together with Theorem 2 immediately imply that the hyper-Wiener index of any n-vertex tree must belong to the interval

$$\left\{\frac{1}{2}(n-1)(3n-4), \frac{1}{24}n(n-1)(n+1)(n+2)\right\}$$

which, in turn, means that WW may assume at most

$$i_n = \frac{1}{24}n(n-1)(n+1)(n+2) - \frac{1}{2}(n-1)(3n-4) + 1$$

distinct numerical values. Evidently, i_n is a quartic polynomial in the variable n.

The number t_n of n-vertex trees is, for instance, found in refs 18 and 19. This number is known[18] to increase much faster than any polynomial.[20] Since for large n t_n is much greater than i_n, it follows that there necessarily must exist large families of trees with equal hyper-Wiener index. In other words, the isomer-discriminating power of the hyper-Wiener index is very weak (at least in the case of large acyclic molecular graphs).

The quantity t_n/i_n is obviously a lower bound for the average size of families of trees with coinciding hyper-Wiener indices. This bound indicates how exceptionally

Table 2. List of Compressed Adjacency Matrices of Trees with $WW = 1895^a$

COL/ROW	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	2	1	3	1	6	1	2	5	10	1	2	1	1	14	10	10	15	7
2	2	3	2	4	3	1	5	8	6	4	8	6	3	1	11	3	15	1
3	2	2	1	1	3	4	4	2	10	8	6	13	10	10	15	16	13	15
4	2	1	1	4	2	3	1	5	9	9	12	10	8	13	10	4	1	3
5	1	2	2	1	3	2	5	3	8	3	8	8	14	6	5	10	7	19
6	1	1	1	2	6	3	4	9	9	3	8	9	14	2	1	5	3	15
7	1	3	4	2	3	7	8	7	1	8	5	10	1	9	4	15	17	7
8	1	1	2	4	2	2	5	4	7	9	8	11	2	3	7	3	18	14
9	1	1	2	2	1	3	4	7	3	11	2	5	14	9	4	11	9	14
10	2	2	3	5	6	2	3	3	10	11	8	12	3	4	7	2	2	16
11	1	2	3	3	3	7	2	4	9	2	6	5	5	14	4	7	5	4
12	2	1	1	5	6	2	6	5	10	10	9	2	8	13	10	5	7	9
13	1	1	3	2	5	1	2	5	6	7	4	5	3	15	6	2	10	13
14	2	2	3	1	2	4	5	4	5	5	1	9	13	1	5	14	16	5
15	1	1	1	3	6	1	1	5	3	1	12	10	3	10	7	16	7	19
16	1	1	1	3	6	1	1	5	3	1	12	10	3	10	7	16	16	19
17	1	2	3	5	4	5	3	9	8	9	1	12	10	3	1	15	17	5
18	2	1	2	5	5	2	2	8	4	7	10	13	13	5	11	1	3	5
19	1	3	1	5	5	6	2	3	5	3	5	1	8	15	4	8	11	9
20	1	2	3	4	2	7	4	1	7	8	11	10	11	7	10	4	18	12
21	2	3	3	5	3	1	7	9	5	1	7	10	9	1	4	5	4	16
22	2	3	3	2	1	1	5	4	7	5	7	3	9	8	11	12	2	2
23	1	1	3	1	1	1	5	5	2	5	2	10	14	2	4	14	17	4
24	2	1	4	2	6	3	1	3	9	5	6	13	4	4	7	4	5	5
25	1	1	3	5	1	5	7	6	1	5	9	1	4	5	15	5	17	18
26	1	2	4	5	6	4	4	1	1	4	7	6	8	2	8	3	5	7
27	2	3	4	4	5	7	1	8	3	5	5	7	2	3	4	11	8	17
28	1	2	1	3	3	2	6	3	2	6	10	9	2	5	9	9	16	16
29	1	1	2	4	4	7	1	7	8	10	11	3	12	7	16	10	18	1
30	1	3	4	3	3	4	5	7	8	10	10	6	5	10	12	3	8	16
31	1	3	4	3	2	4	2	4	7	3	1	12	5	3	16	10	7	19
32	2	3	4	2	1	6	7	1	2	6	9	3	9	11	1	14	4	9
33	2	1	2	4	4	1	2	4	8	5	2	6	14	5	1	16	11	14
34	1	1	2	4	6	1	7	1	9	2	6	10	12	8	16	4	4	16
35	2	2	2	3	5	6	5	6	6	11	2	12	2	11	10	17	13	4
36	2	3	2	5	4	5	1	5	10	5	6	1	5	4	16	11	11	1
37	2	2	1	4	2	7	8	6	8	2	11	3	12	8	1	11	6	17
38	2	1	2	4	3	6	4	9	2	10	9	6	1	10	5	9	18	6
39	1	1	1	5	3	1	8	3	5	5	4	9	14	7	11	5	16	17
40	1	2	2	5	2	4	5	1	8	2	12	11	7	8	7	16	3	19
41	2	2	2	5	3	3	8	1	6	10	4	7	10	7	4	1	12	18
42	1	3	3	5	6	7	7	1	4	3	1	10	3	6	15	12	4	8
43	2	3	2	4	3	1	2	9	10	6	10	8	1	5	6	1	18	3
44	1	2	4	3	6	7	3	2	9	3	1	1	12	4	10	4	7	13
45	2	3	4	4	4	4	2	1	8	2	7	13	3	6	7	1	18	17
46	1	2	1	2	1	5	7	5	4	11	3	1	8	8	2	12	15	5
47	1	3	3	1	3	3	2	8	5	5	4	11	9	10	5	12	15	8
48	1	2	3	1	2	7	4	7	2	9	11	5	2	10	6	8	11	12
49	1	2	3	2	6	4	3	3	8	1	10	2	2	9	16	13	9	2
50	2	3	4	1	4	3	8	2	6	4	3	9	6	12	3	17	18	18

[a] Entries denote the row numbers, which with the corresponding column number give the nonzero matrix element $A_{i,j}$.

large isomer-degeneracy of the hyper-Wiener index is to be expected. Table 1 provides the respective numerical values. In Table 1 we have included also the exact values (F_n) for the average size of families of n-vertex trees with equal hyper-Wiener indices.[21] The agreement between t_n/i_n and F_n is remarkably good, especially for large values of n. From Table 1 we see that until $n = 10$ the isomer-degeneracy is not large. Already at $n = 14$ more than three trees (or, according to our lower bound: more than two trees) *in average* have equal WW. At $n = 20$ finding 160-membered families of trees with equal WW would be rather a rule than an exception. At 23 such average families have well over 1000 members.

The fact that several trees have identical graph invariants (here WW) is of interest not because of the isomorphism testing (as nobody today expects that a single simple invariant can do that) but more as an indicator of the extent of loss of structural information that accompanies the respective invariant. For that purpose it is of interest to know what is the size of the smallest graphs showing degeneracy.

By direct calculation we established that up to $n = 8$ there are no two n-vertex trees with the same hyper-Wiener index. There are, however, four pairs of 9-vertex trees and two triplets of 10-vertex trees with coinciding WW. For $n = 11$, 12, 13, ..., 23 the maximal sizes of such families are 4, 6, 10, 17, 26, 50, 86, 160, 319, 657, 1391, 3184, and 6714, respectively. These maximal families are unique, except for $n = 12$, where there are two series of six trees with equal WW.

The isomer-discriminating power of the hyper-Wiener index (and to an even higher extent, of the Wiener index[22−24]) is therefore clearly insufficient for documentary purposes. On the other hand, many investigations concerning the utility of W and WW in a series of isomeric hydrocarbons indicate that these indices—especially when combined with p (the number of distances equal to three) and other similar structural invariants[25]—are highly important parameters in quantitative structure-property relationships. The indices W and WW could be correlated with a number of physical properties of hydrocarbons. We have no reason to assume that W and WW will not function in QSPRs, done for a series of heavier hydrocarbon isomers. We therefore expect that it will be increasingly difficult to separate higher hydrocarbon isomers because of their rather similar physical properties.

GENERATION OF TREES WITH IDENTICAL HYPER-WIENER INDICES

The adjacency matrix $\mathbf{A} = ||A_{i,j}||$ has n rows and n columns; $A_{i,j} = 1$ if and only if vertices i and j are joined by an edge, and $A_{i,j} = 0$ otherwise.[26,27] A random generation of the adjacency matrix **A** was done in order to find trees with $n = 20$ and a prescribed value of WW. We constructed random adjacency matrices of 20-vertex trees, in which there is only one nonzero entry in every column of the upper off-diagonal triangle.[28]

We have chosen $WW = 1895$ as the prescribed value. This figure was obtained by drawing by random a tree with $N = 20$ and calculating its WW-value. It happened that the result $WW = 1895$ was obtained.

Therefore there is at least one 20-vertex tree with $WW = 1895$. From the considerations in the preceding section we know that it is very likely (although by no means certain) that there will be more trees with the same hyper-Wiener index.

If the WW-value pertaining to a randomly generated adjacency matrix[29] was not equal to the prescribed value, the next adjacency matrix was generated. If WW was equal to the prescribed value, then the following structure-descriptors,[28] the Wiener index W, Randić's connectivity index χ, and Balaban's index J, were computed and subsequently compared with the respective indices of the trees that already belonged to the set. The new tree was added to the set (i.e., accepted) only if at least one of its indices W, χ, and J differed from the same triplet of indices of each member of the set. In this way we were sure that no two mutually isomorphic trees were chosen. There is a possibility that nonisomorphic trees with coinciding WW, W, χ, and J values were generated by our procedure, in which case only one of them was included into the set.

The generation was performed on an IBM AT-486 PC. Fourteen hours were necessary for generation of 200 000 adjacency matrices. As a result we obtained adjacency matrices of 50 nonisomorphic trees with $WW = 1895$. It has to be noted that the generation was not complete; in fact many more trees with $n = 20$ and $WW = 1895$ may exist.

In Table 2 the adjacency matrices are listed in a compressed form. In this list each row denotes a matrix. The entries indicate the row index i, which together with the corresponding column denote the nonzero element of the upper off-diagonal triangle of the matrix **A**. Note that $A_{1,2} = 1$ in all cases and therefore it is not listed in Table 2. The first column in Table 2 corresponds therefore to column 3 of the adjacency matrix. For instance, in row 1 the third entry is equal to 3, indicating that $A_{3,5} = 1$ and that there is no other unit entry in the fifth column of the upper triangle. From Table 2 the underlying trees are directly reconstructed.

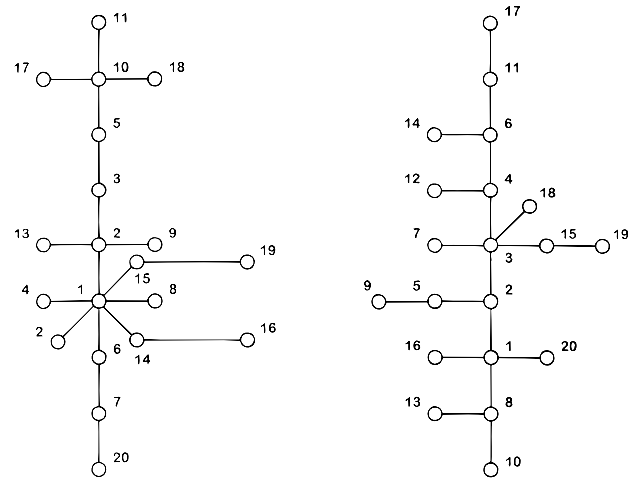

Figure 3. Two trees with $WW = 1895$ corresponding to the first two rows of Table 2.

For example, Figure 3 shows the trees corresponding to the first two rows of Table 2.

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(16) Equations 6 and 12 should be compared with the analogous expressions for the Wiener index[12,13] $W(S_n) = (n-1)^2$ and $W(P_n) = {}^1/_6 n(n-1)(n+1) = [(n+1)/3]$.

(17) We mention in passing the identities $WW(S_n) = {}^3/_2 W(S_n) - {}^1/_2\sqrt{W(S_n)}$ and $WW(P_n) = WW(P_{n-1}) + W(P_n)$.

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(20) The number t_n of n-vertex trees increases with n only slightly slower than an exponential function. For large enough n the following asymptotic relation holds (see page 214 of ref. 16): $t_n = AB^n n^{-5/2} + O(B^n n^{-7/2})$, where $A \approx 0.535$ and $B \approx 2.9558$.

(21) The calculation of the quantity F_n in Table 1 requires the computation of the WW-values of all n-vertex trees. Therefore we obtained F_n only up to $n = 23$. Calculations for larger values of n are hardly worth the effort, in view of the good agreement between f_n and F_n.

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(28) In order that there is only one nonzero entry in every column of the upper off-diagonal triangle of the adjacency matrix of a tree, the vertices of the tree have to be labeled according to the following recipe: Choose any vertex and label it by 1. For i=2, ..., n choose a vertex whose first neighbor has already been labeled and label this vertex by i. Clearly, the labeling obtained by the above recipe is not unique. Figure 3 shows one of the many possible labelings of this kind.

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