# Simple Construction of Embedding Frequencies of Trees and Rooted Trees

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A unified approach for the calculation of embedding frequencies of trees as well as rooted trees is suggested. It consists of a simple pruning process when marginal vertices are successively removed. The problem of isomorphism between (rooted) trees is solved by making use of Read's linear canonical code. Simple criteria, based on the concept of valence vectors, for verification whether a (rooted) tree can be a subtree of a (rooted) tree are proved. Tables of embedding frequencies of trees and rooted trees through ten and eight vertices, respectively, are presented. The embedding frequencies of rooted trees are useful for construction of descriptors of molecular graphs when the so-called local properties are studied.

## INTRODUCTION

Graph-theoretic cluster expansion1-6 of physical and chemical properties of molecular systems represented by structural formulae belongs to very promising approaches on how to study structure-activity and/or structure-property relationships. This approach is usually based on the so-called embedding frequencies<sup>1,2,7-10</sup> which are determined, loosely speaking, as numbers of time a given submolecular cluster (subgraph) appears as a subgraph in the molecular graph (a formal representation of structural formula). Poshusta and McHughes9 have suggested an algorithm for finding embedding frequencies of subtrees in a given larger tree. They published an extensive list of all embedding frequencies of trees through ten vertices. In the paper<sup>10</sup> they demonstrated efficiency of this approach for a prediction of thermochemical properties of alkanes. The values of these properties may be with high precision expressed as linear combinations of embedding frequencies assigned to few smaller subtrees. Magnetic susceptibility, which can be computed by "additive" graph-theoretical cluster expansion in terms of molecular fragments, can serve as another example of a special type of property.<sup>11</sup> Such properties may be formally considered as global properties, a given property is strongly dependent on the whole structure of molecular graphs. Another group of molecular properties is classified as local properties. Here, it is possible to assign the given property to an atom (vertex) of structural formula (molecular graph). The very instructive example of these properties are <sup>13</sup>C NMR chemical shifts of alkanes; they are unambiguously assigned (up to symmetry) to single carbon atoms of alkane skeletons. In order to correlate the local properties with the structure of molecular graphs we have to know information about the environment of the given vertex. The chosen atom plays a role of the so-called root, 12 a vertex distinguished from other vertices of the molecular graph. Therefore, if we would like to use the graph-theoretic cluster expansion for local molecular properties, then the embedding frequencies of rooted subgraphs in the given larger rooted graph should be known. This graph-theoretic problem corresponds to a special case of the original approach of embedding frequencies, the rooted graphs are more restricted forms of trees with one vertex distinguished from other ones.

The purpose of this paper is to outline a unified approach for the calculation of embedding frequencies of trees as well as rooted trees. We shall prove simple criteria, based on the so-called *valence vectors*, whether a given (rooted) tree can be a (rooted) subtree of a larger (rooted) tree. If one of those criteria is not satisfied, then the relationship "to be subtree" is falsified. A simple pruning process consisting of successively removing marginal vertices (with unit valences) is suggested. Its application allows us to construct in a simple way the embedding frequencies of (rooted) trees. An algorithm of the pruning process in a backtrack form is suggested.

Two extensive tables of embedding frequencies are presented. The first table lists embedding frequencies of smaller *trees* through five vertices in larger trees through ten vertices. The trees are identified by Read's linear codes in canonical form, <sup>13</sup> where the subcodes are ordered in a lexicographically nonincreasing sequence. This canonicity of codes ensures their uniqueness for forthcoming applications of embedding frequencies. Unfortunately, in Poshusta and McHughes' papers<sup>9</sup> the codes of trees they used are not presented in the canonical form (e.g., the tree no. 53 coded as 221010200 has the canonical code 220021010), therefore in some cases utilization of their results may involve serious difficulties.

The second table lists embedding frequencies of smaller rooted trees through five vertices in larger rooted trees through eight vertices; similarly, as in the first table, rooted trees are coded canonically.

The used code for trees is certainly not the only useful code; a nice example of code, which does not necessarily need separation for vertices with a degree higher then 10, is presented in ref 14. Plans for embedding search of rooted trees were suggested already in ref 15. The very idea of characterization of trees by embeddings even found its implementation in Gordon—Scantlebury topological index, which equals the number of embeddings of propan skeleton, and also a "centric topological index" was devised on the basis of the prunning process. <sup>16</sup>

## **THEORY**

Let us consider a  $tree^{12}$  (connected nonoriented graph without cycles) T = (V,E), where  $V = \{v_1,v_2,...,v_N\}$  is a nonempty (i.e.,  $N \ge 1$ ) vertex set and  $E = \{e_1,e_2,...,e_M\}$  is

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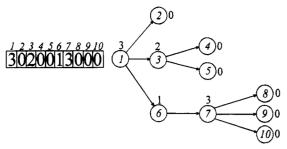


Figure 1. Illustrative example of the linear code of trees, with its entries labeled by integers (placed above them) corresponding to their sequential numbers. Reading the code from the left- to the right-hand side we may simply reconstruct the coded tree. Each entry determines the number of vertices attached from the right hand-side to the corresponding vertex. The vertices of trees are represented by open circles with vertex indices (sequential numbers of code) placed inside.

an edge set. The cardinalities of sets V and E are mutually related by

$$M = N - 1 \tag{1}$$

Let  $v \in V$  be a vertex of the tree T: the valence or degree of this vertex, denoted by val(v), is the number of edges that are incident with the vertex v. The sum of valences of all vertices satisfies  $^{12}$ 

$$\sum_{v \in V} \text{val}(v) = 2M = 2(N - 1)$$
 (2)

A rooted tree<sup>12</sup> has one vertex, called the *root*, which is especially distinguished from the vertices of V. Formally, the rooted tree will be determined as an ordered triple

$$T(v) = (V, E, v) \tag{3}$$

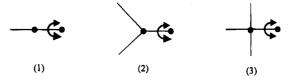
where  $v \in V$  is the root of the rooted tree T(v). Two rooted trees T(v) = (V, E, v) and T'(v') = (V', E', v') are isomorphic<sup>12</sup>  $(T(v) \approx T'(v'))$  if and only if there exists a one-to-one mapping  $\phi: V \to V'$  which saves the adjacency of vertices and maps the root of T(v) onto the root of T'(v'), i.e.,  $\phi(v) = v'$ .

Carbon skeletons of alkanes may be represented by trees, which are composed of vertices with valences bounded by  $1 \le \text{val}(v) \le 4$ , for  $\forall v \in V$ . The vertices with unit valences are called *marginal vertices* or *endpoints*. In our forthcoming considerations we shall restrict ourselves to trees which correspond to alkanes, i.e., to trees with vertex valences equal at most to four. For (rooted) trees each subtree must be the so-called *induced subgraph*. This means that a verification of  $T \subseteq T$  (T is a subtree of T) is reduced to a finding of the subset  $V \subseteq V(T)$  so that a subtree induced by V is isomorphic to the tree T. Moreover, if  $T \subseteq T$  and |V(T')| = |V(T)|, then trees T and T' are isomorphic.

An isomorphism between two (rooted) trees may be simply verified by making use of the linear code extensively studied by Read<sup>13</sup> and Knop et al., <sup>17,18</sup> see Figure 1. This type of linear code is endowed by the very important property that two (rooted) trees are isomorphic if and only if their codes are identical.

We assign to each (rooted) tree T an ordered four-tuple (called the *valence vector*) composed of nonnegative integer entries

$$v_T = (v_1, v_2, v_3, v_4) \tag{4}$$



**Figure 2.** All three possible events that can appear when a marginal vertex is removed from a tree. The corresponding changes of valence vectors are specified by (7) and/or (8).

where  $v_i$  (for i = 1,2,3,4) is the number of vertices of T with valence equal to i. The entries of (4) satisfy the following two conditions (see eqs 1 and 2)

$$\sum_{i=1}^{4} v_i = N \tag{5a}$$

$$\sum_{i=1}^{4} i v_i = 2M = 2(N-1)$$
 (5b)

These two conditions together are not only necessary but also sufficient for the valence vector  $v_T$  to be graphable, 12 that is there exists a (rooted) tree T with the valence vector  $v_T = (v_1, v_2, v_3, v_4)$ .

Let us have two (rooted) trees T' and T that are related by  $T' \subseteq T$ ; their valence vectors are denoted by  $v_T = (v_1', v_2', v_3', v_4')$  and  $v_T = (v_1, v_2, v_3, v_4)$ , respectively, then

$$\sum_{i=p}^{4} (v_i' - v_i) \le 0 \tag{6a}$$

$$\sum_{i=1}^{p} (v_i' - v_i) \le 0 \tag{6b}$$

for p = 1,2,3,4.

Applying these requirements we may simply verify whether a (rooted) tree T can be a subtree of T. If there exists  $1 \le p \le 4$  so that one of (or both) inequalities (16) are not satisfied, then T could not be a subtree of T. Its proof can be done in a simple way as follows. Let us consider a marginal vertex (except the root for rooted trees) of T: removing this marginal vertex from T we arrive at a new (rooted) tree T with valence vector determined by three alternative ways (see Figure 2)

case 1: 
$$v_T = (v_1, v_2 - 1, v_3, v_4)$$
  
case 2:  $v_T = (v_1 - 1, v_2 + 1, v_3 - 1, v_4)$  (7)  
case 3:  $v_T = (v_1 - 1, v_2, v_3 + 1, v_4 - 1)$ 

The difference  $\Delta v = v_T - v_T$  is determined by

case 1: 
$$\Delta v = (0,-1,0,0)$$
  
case 2:  $\Delta v = (-1,1,-1,0)$  (8)  
case 3:  $\Delta v = (-1,0,1,-1)$ 

It is easy to verify that for all three cases the requirements (6a,b) are satisfied. But this was proved only for trees  $T \subset T$  such that T is created from T removing a marginal vertex. For a general pair  $T \subset T$  these properties should be also satisfied, since the tree T may be formed from T by a

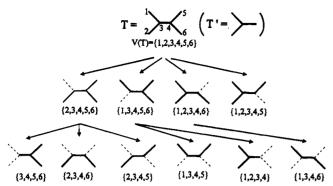


Figure 3. Outline of the pruning process for finding the embedding frequency n(T,T), both trees are displayed at the top of the figure. First, we remove successively all marginal vertices of T, to obtain four subtrees that are displayed together with their vertex subsets in the second row of figure. Second, the pruning process is repeated for the subtrees obtained in the previous step. The algorithm produces only subtrees induced by different vertex subsets. Only two subtrees (the first and the last but one) satisfy conditions (6a,b) and are isomorphic to T, so that the embedding frequency of T in T is n(T,T')=2.

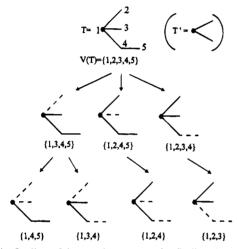


Figure 4. Outline of the pruning process for finding the embedding frequency n(T,T') of the rooted subtree T' in the rooted tree T. The approach is the same as in Figure 3, but the root is never removed in the process of pruning. From the third row of figure we see that the embedding frequency is n(T,T') = 3.

successive removing of marginal vertices. We get a sequence  $T_0 = T' \subset T_1 \subset ... \subset T_n = T$  so that for each pair  $T_{i-1} \subset T_i$ (for i = 1,2,...,n) the above conditions are satisfied, hence they should be also satisfied for  $T' \subset T$ , as was to be proved.

We turn now our attention to the construction of vertex subsets  $\tilde{V} \subset V(T)$ , which induce subtrees isomorphic to the prescribed (rooted) tree T'. The following pruning process forms all possibilities that will give the subset  $\tilde{V}$ . This vertex subset may be constructed by successive removal of a marginal vertex (except the root for rooted trees) from the current vertex subset, and a new vertex subset is formed. By further use of the described backtrack algorithm, it is ensured that this new subset has not been already formed in the previous steps. If the cardinality of the current subset  $\tilde{V}$ is equal to the cardinality of the vertex set of the subtree T, then we construct the canonical code of a subtree  $T(\tilde{V})$ induced by  $\tilde{V}$ . The equality of codes of T' and  $T(\tilde{V})$  implies that these (rooted) trees are isomorphic. The pruning process can be substantially accelerated by applying requirements (6). If one of them is not satisfied, then the current branch of pruning is stopped due to the fact that the property

 $T \subset T(\tilde{V})$  could not be fulfilled. Simple illustrative examples of the pruning processes for trees as well as rooted trees are displayed in Figures 3 and 4, respectively.

The embedding frequency of a (rooted) subtree T' in a (rooted) tree T, denoted by n(T,T'), may now be defined as the number of appearances of vertex subsets  $\tilde{V} \subset V(T)$  in the pruning process such that the (rooted) subtree induced by  $\tilde{V}$ is isomorphic to the (rooted) subtree T. The embedding frequencies of all trees up to ten vertices have been tabulated by Poshusta and McHughes.<sup>9</sup> The above outlined simple algorithm for constructing embedding frequencies based on the pruning process has been checked by Poshusta's results, with perfect agreement having been achieved. A pseudo-Pascal code of the pruning algorithm specified above in a form of the backtrack searching looks as follows.

#### Pruning algorithm

```
V<sub>s</sub>:=V(T); U<sub>s</sub>:={marginal vertices of T}; k:=1;
1
        C_i := \{V_i\}; for i := 1 to |V(T)| - 1 do C_i := \sigma;
3
        while k>0 do
        if |U_|>0 then
        begin v:=an element of U;
               U_:=U_\{v}; A:=V___\\{v};
7
               begin C_i := C_i \cup \{A\}; V_i := A; k := k+1;
                       8
               end;
10
         end else k:=k-1;
```

The first two lines initialize the algorithm. The integer variable k determines the so-called depth of searching. The set  $V_k$  is a current vertex subset and the set  $U_k$  is composed of marginal vertices of the subtree induced by  $V_{k-1}$  such that these marginal vertices have not been used yet in previous levels in the backtrack searching. The class  $C_k$  is composed of all possible different vertex subsets that have been constructed for the depth k. The system of inequalities (6a,b) may be applied in line 7, i.e., class  $C_k$  is enlarged only if the subgraph satisfies these inequalities. If one of them is not satisfied, then the current branch of the search tree is stopped, and the while cycle (line 3) is repeated for a new marginal vertex v.

Let us calculate the embedding frequency n(T,T'), where  $T \subset T$  (this property may be verified by conditions (6a,b)), |V(T)| = N, |V(T')| = N', and  $N' \le N$ . For k = N - N' we construct all (rooted) trees that are induced by vertex subsets of  $C_k$ , then the embedding frequency n(T,T') is equal to the number of all induced (rooted) trees that are isomorphic with T'.

In Table 1 are listed all embedding frequencies of trees through ten vertices and in Table 2 all embedding frequencies of rooted trees through eight vertices. The embedding frequencies of all trees through ten vertices are calculated for all possible eight subtrees through five vertices, see Figure 5. Similarly, the embedding frequencies of all rooted trees through eight vertices are calculated for all possible 17 rooted subtrees (see Figure 6) through five vertices; though we have omitted the rooted subtree composed of one vertex (i.e., root). its embedding frequency for each rooted tree automatically being equal to 1.

Table 1. Embedding Frequencies of All Trees through Ten Vertices

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51 9 21 220103000 9 8 11 7 5 7 5 1 224MMM-C6 136 10 61 4002001110 10 9 12 11 5 6 12 1 233MMM-C7 62 9 22 230003000 9 8 13 6 8 9 6 2 2244MMMM-C5 137 10 62 4002001200 10 9 13 11 6 8 13 1 2335MMMM-C6 63 9 23 400101110 9 8 10 8 4 5 6 1 33MM-C7 138 10 63 3011030010 10 9 12 12 5 7 13 1 334MMM-C7 65 9 25 400101200 9 8 11 8 5 7 7 1 244MMM-C6 140 10 65 3101030010 10 9 12 12 5 8 13 1 344MMM-C7 65 9 25 400101200 9 8 11 8 5 7 7 1 244MMM-C6 140 10 65 3101030010 10 9 12 13 5 9 14 1 334MMM-C6 65 9 26 401010110 9 8 10 10 4 6 9 1 33EM-C6 141 10 66 3020030010 10 9 13 13 6 8 16 1 2344MMMM-C6 65 9 27 410101010 9 8 10 12 4 6 12 1 33EM-C6 141 10 66 3020030010 10 9 13 13 6 8 16 1 2344MMMM-C6 65 9 28 301103000 9 8 11 1 9 5 5 10 1 223MMM-C6 143 10 68 4010102010 10 9 12 13 5 8 15 1 233MME-C6 65 9 29 310103000 9 8 11 10 5 7 11 1 223MME-C5 144 10 69 4101010200 10 9 12 15 5 9 18 1 332EEM-C5 70 9 30 302003000 9 8 12 10 6 6 13 1 2234MMMM-C5 145 10 70 4002002010 10 9 13 15 6 8 21 1 2334MMM-C6 71 9 31 400110200 9 8 11 10 5 5 12 1 233MMM-C6 146 10 71 4010200200 10 9 13 15 6 8 21 1 2334MMMM-C6 73 9 33 401010200 9 8 11 11 5 5 13 1 334MMM-C6 147 10 72 4001103000 10 9 14 13 8 6 21 2 2233MMMM-C6 74 9 34 400200200 9 8 12 12 6 4 18 1 2334MMMM-C5 149 10 74 4010103000 10 9 14 15 8 7 24 2 3223EMMM-C6 74 9 34 400200200 9 8 12 12 6 4 18 1 2334MMMM-C5 149 10 74 4010103000 10 9 14 15 8 7 24 2 3223EMMM-C5																												
52 9 22 230003000 9 8 13 6 8 9 6 2 2244MMMM-C5 137 10 62 4002001200 10 9 13 11 6 8 13 1 2335MMMM-C6 63 9 23 400101110 9 8 10 8 4 5 6 1 33MM-C7 138 10 63 3011030010 10 9 12 12 5 7 13 1 334MMM-C7 64 9 24 400110110 9 8 10 8 4 7 6 1 44MM-C7 139 10 64 4001102010 10 9 12 12 5 8 13 1 344MMM-C7 65 9 25 400101200 9 8 11 8 5 7 7 1 244MMM-C6 140 10 65 3101030010 10 9 12 12 5 8 13 1 344MMM-C7 65 9 26 40101010 9 8 10 10 4 6 9 1 33EB-C5 142 10 66 3020030010 10 9 12 13 5 9 14 1 334MMB-C6 65 9 27 410101010 9 8 10 12 4 6 12 1 33EB-C5 142 10 67 4010110200 10 9 12 13 5 8 15 1 233MMB-C6 65 9 28 301103000 9 8 11 9 5 5 10 1 223MMM-C6 143 10 68 4010102010 10 9 12 13 5 8 15 1 233MMB-C6 65 9 29 310103000 9 8 11 10 5 7 11 1 223MMB-C5 144 10 69 4101010200 10 9 12 15 5 9 18 1 332EBM-C5 67 9 30 302003000 9 8 12 10 6 6 13 1 2234MMMM-C5 145 10 70 4002002010 10 9 13 14 6 7 19 1 2334MMMM-C6 67 9 31 400110200 9 8 11 10 5 5 12 1 233MMB-C6 146 10 71 4010200200 10 9 13 15 6 8 21 1 3234EMMMM-C6 67 9 32 400102010 9 8 11 11 5 5 13 1 334MMM-C6 147 10 72 4001103000 10 9 14 15 8 6 24 2 2233MMMM-C6 67 9 33 400102000 9 8 11 11 2 5 5 15 1 233MMB-C5 148 10 73 400103000 10 9 14 15 8 6 24 2 2333MMM-C6 67 9 34 400200200 9 8 12 12 6 4 18 1 2334MMMM-C5 149 10 74 4010103000 10 9 14 15 8 7 24 2 3223EMMM-C5																												
53 9 23 400101110 9 8 10 8 4 5 6 1 33MM-C7 138 10 63 3011030010 10 9 12 12 5 7 13 1 334MMM-C7 65 9 24 400110110 9 8 10 8 4 7 6 1 44MM-C7 139 10 64 4001102010 10 9 12 12 5 8 13 1 344MMM-C7 65 9 25 400101200 9 8 11 8 5 7 7 1 244MMM-C6 140 10 65 3101030010 10 9 12 13 5 9 14 1 334MME-C6 65 9 26 401010110 9 8 10 10 4 6 9 1 33EE-C5 142 10 67 4010110200 10 9 12 13 5 8 16 1 2344MMM-C6 65 9 28 301103000 9 8 11 10 5 7 11 1 223MME-C5 142 10 67 401010200 10 9 12 13 5 8 16 1 343MME-C6 65 9 29 310103000 9 8 11 10 5 7 11 1 223MME-C5 144 10 69 4101010200 10 9 12 15 5 9 18 1 332EEM-C5 142 10 67 401010200 10 9 12 15 5 9 18 1 332EEM-C5 142 10 67 402002010 10 9 12 15 5 9 18 1 332EEM-C5 142 10 67 401010200 10 9 12 15 5 9 18 1 332EEM-C5 142 10 67 401010200 10 9 12 15 5 9 18 1 332EEM-C5 142 10 67 401010200 10 9 12 15 5 9 18 1 332EEM-C5 144 10 69 4101010200 10 9 12 15 5 9 18 1 332EEM-C5 142 10 67 401010200 10 9 12 15 5 9 18 1 332EEM-C5 142 10 67 401010200 10 9 12 15 5 9 18 1 332EEM-C5 142 10 67 401010200 10 9 13 15 6 8 21 1 3234MMMM-C6 146 10 71 4010200200 10 9 13 15 6 8 21 1 3234MMMM-C6 147 10 72 4001103000 10 9 14 15 8 6 21 2 2233MMMM-C6 147 10 72 4001103000 10 9 14 15 8 6 24 2 3233MMMM-C6 147 10 73 400103000 10 9 14 15 8 6 24 2 3334MMM-C6 147 10 73 400103000 10 9 14 15 8 6 24 2 3334MMM-C6 147 10 74 4010103000 10 9 14 15 8 6 24 2 3334MMM-C6 147 10 74 4010103000 10 9 14 15 8 6 24 2 3334MMM-C6 147 10 74 4010103000 10 9 14 15 8 6 24 2 3334MMM-C6 147 10 74 4010103000 10 9 14 15 8 6 24 2 3334MMM-C6 148 10 73 400103000 10 9 14 15 8 6 24 2 3334MMM-C6 148 10 73 400103000 10 9 14 15 8 7 24 2 3223EMMM-C5 148 10 73 400103000 10 9 14 15 8 7 24 2 3223EMMM-C5 149 10 74 4010103000 10 9 14 15 8 7 24 2 3223EMMM-C5 149 10 74 4010103000 10 9 14 15 8 7 24 2 3223EMMM-C5 149 10 74 4010103000 10 9 14 15 8 7 24 2 3223EMMM-C5 149 10 74 4010103000 10 9 14 15 8 7 24 2 3223EMMM-C5 149 10 74 4010103000 10 9 14 15 8 7 24 2 3223EMMM-C5 149 10 74 4010103000 10 9 14 15 8 7 24 2 3223EMMM-C5 149 10 74 4010103000 10 9 14 15 8 7 24 2 3223EMMM-C5 149 10 74 4010103000 10																												
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56 9 26 401010110 9 8 10 10 4 6 9 1 33EM-C6 141 10 66 3020030010 10 9 13 13 6 8 16 1 2344MMMM-C6 57 9 27 410101010 9 8 10 12 4 6 12 1 33EE-C5 142 10 67 4010110200 10 9 12 13 5 8 15 1 233MME-C6 58 9 28 301103000 9 8 11 1 9 5 5 10 1 223MMM-C6 143 10 68 401010201 10 9 12 14 5 8 16 1 343MME-C6 59 9 29 310103000 9 8 11 10 5 7 11 1 223MMM-C5 144 10 69 4101010200 10 9 12 15 5 9 18 1 332EEM-C5 70 9 30 302003000 9 8 12 10 6 6 13 1 2234MMMM-C5 145 10 70 4002002010 10 9 12 15 5 9 18 1 332EEM-C5 71 9 31 400110200 9 8 11 10 5 5 12 1 233MMM-C6 147 10 72 4001103000 10 9 13 15 6 8 21 1 3234MMMM-C6 72 9 32 400102010 9 8 11 11 5 5 13 1 334MMM-C6 147 10 72 4001103000 10 9 14 13 8 6 21 2 2233MMMM-C6 73 9 33 401010200 9 8 11 12 5 5 15 1 233MMM-C5 148 10 73 400103000 10 9 14 15 8 6 24 2 3344MMMM-C6 74 9 34 400200200 9 8 12 12 6 4 18 1 2334MMMM-C5 149 10 74 4010103000 10 9 14 15 8 7 24 2 3223EMMM-C5																	4001102010	10	9	12	12	5						
57 9 27 410101010 9 8 10 12 4 6 12 1 33EE-C5 142 10 67 4010110200 10 9 12 13 5 8 15 1 233MME-C6 58 9 28 301103000 9 8 11 1 9 5 5 10 1 223MMM-C6 144 10 69 4101010200 10 9 12 15 5 9 18 1 332EEM-C5 70 9 30 302003000 9 8 12 10 6 6 13 1 2234MMMM-C5 145 10 70 4002002010 10 9 12 15 5 9 18 1 332EEM-C5 71 9 31 400110200 9 8 11 10 5 5 12 1 233MMM-C6 146 10 71 4010200200 10 9 13 15 6 8 21 1 3234MMMM-C6 73 9 32 400102010 9 8 11 11 5 5 13 1 334MMM-C6 147 10 72 4001103000 10 9 14 13 8 6 21 2 2233MMMM-C6 73 9 33 401010200 9 8 12 12 6 4 18 1 233MMM-C5 149 10 74 4010103000 10 9 14 15 8 6 24 2 334MMMM-C6 74 9 34 40020200 9 8 12 12 6 4 18 1 2334MMMM-C5 149 10 74 4010103000 10 9 14 15 8 7 24 2 3223EMMM-C5																												
58 9 28 301103000 9 8 11 9 5 5 10 1 223MMM-C6 59 9 29 310103000 9 8 11 10 5 7 11 1 223MME-C5 144 10 69 4101010200 10 9 12 14 5 8 16 1 343MME-C5 70 9 30 302003000 9 8 12 10 6 6 13 1 2234MMMM-C5 145 10 70 4002002010 10 9 12 15 5 9 18 1 332EEM-C5 71 9 31 400110200 9 8 11 10 5 5 12 1 233MMM-C6 146 10 71 4010200200 10 9 13 14 6 7 19 1 2334MMMM-C6 72 9 32 400102010 9 8 11 11 5 5 13 1 334MMM-C6 147 10 72 4001103000 10 9 14 13 8 6 21 2 2233MMMM-C6 73 9 33 401010200 9 8 11 12 5 5 15 1 233MME-C5 148 10 73 400103001 10 9 14 15 8 6 24 2 3344MMMM-C6 74 9 34 400200200 9 8 12 12 6 4 18 1 2334MMMM-C5 149 10 74 4010103000 10 9 14 15 8 7 24 2 3223EMMM-C5																							8	15	1	233MME-C6		
59 9 29 310103000 9 8 11 10 5 7 11 1 223MME-C5 144 10 69 4101010200 10 9 12 15 5 9 18 1 332EEM-C5 70 9 30 302003000 9 8 12 10 6 6 13 1 2234MMMM-C5 145 10 70 4002002010 10 9 13 14 6 7 19 1 2334MMMM-C6 71 9 31 400110200 9 8 11 10 5 5 12 1 233MMM-C6 146 10 71 4010200200 10 9 13 15 6 8 21 1 3234EMMM-C5 72 9 32 400102010 9 8 11 11 5 5 13 1 334MMM-C6 147 10 72 4001103000 10 9 14 13 8 6 21 2 2233MMMM-C6 73 9 33 401010200 9 8 11 12 5 5 15 1 233MME-C5 148 10 73 4001030010 10 9 14 15 8 6 24 2 3344MMMM-C6 74 9 34 400200200 9 8 12 12 6 4 18 1 2334MMMM-C5 149 10 74 4010103000 10 9 14 15 8 7 24 2 3223EMMM-C5																	4010102010	10	9	12	14	5	8					
70 9 30 302003000 9 8 12 10 6 6 13 1 2234MMMM-C5 145 10 70 4002002010 10 9 13 14 6 7 19 1 2334MMMM-C6 71 9 31 400110200 9 8 11 10 5 5 12 1 2334MMM-C6 146 10 71 4010200200 10 9 13 15 6 8 21 1 3234EMMM-C5 72 9 32 400102010 9 8 11 11 5 5 13 1 334MMM-C6 147 10 72 4001103000 10 9 14 13 8 6 21 2 2233MMMM-C6 73 9 33 401010200 9 8 11 12 5 5 15 1 2334MMM-C5 148 10 73 400103001 10 9 14 15 8 6 24 2 3344MMMM-C6 74 9 34 400200200 9 8 12 12 6 4 18 1 2334MMMM-C5 149 10 74 4010103000 10 9 14 15 8 7 24 2 3223EMMM-C5				310103000	9	8	11	10	5	7 1	1	22:	3MME-C5	144	10	69	4101010200	10	9	12	15	5	9	18	1	332EEM-C5		
72 9 32 400102010 9 8 11 11 5 5 13 1 334MMM-C6 147 10 72 4001103000 10 9 14 13 8 6 21 2 2233MMMM-C6 73 9 33 401010200 9 8 11 12 5 5 15 1 233MME-C5 148 10 73 400103001 10 9 14 15 8 6 24 2 3344MMMM-C6 74 9 34 400200200 9 8 12 12 6 4 18 1 2334MMMM-C5 149 10 74 4010103000 10 9 14 15 8 7 24 2 3223EMMM-C5				302003000	9	8	12	10	6	6 13	3 1	22:	34MMMM-C5				4002002010	10	9	13	14	6	7					
73 9 33 401010200 9 8 11 12 5 5 15 1 233MME-C5 148 10 73 4001030010 10 9 14 15 8 6 24 2 3344MMMM-C6 74 9 34 400200200 9 8 12 12 6 4 18 1 2334MMMM-C5 149 10 74 4010103000 10 9 14 15 8 7 24 2 3223EMMM-C5																							8	21	1	3234EMMM-C5		
74 9 34 400200200 9 8 12 12 6 4 18 1 2334MMMM-C5 149 10 74 4010103000 10 9 14 15 8 7 24 2 3223EMMM-C5																	4001103000	10	9	14	15	8	6	24	2	3344MMMM-C6		
75 9 35 400103000 9 8 13 12 8 3 21 2 2233MMMM-C5 150 10 75 4002003000 10 9 15 15 9 6 27 2 22334MMMMM-C																	4010103000	10	ģ	14	15	8	7	24	2	3223EMMM-C5		
				400103000	9	8	13	12	8	3 2	2	22	33MMMM-C5	150	10	75	4002003000	10	9	15	15	9	6	27	2	22334MMMMMM-C		

<sup>&</sup>lt;sup>a</sup> Serial number of trees with fixed number of vertices (see second column). <sup>b</sup> Names of alkanes are constructed after refs 14 and 29.

Table 2. Embedding Frequencies of All Rooted Trees through Eight Vertices

			embedding frequencies																
no.	N	no.a	code	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	2	1 1	10 110	1 1	0 1	0	0	0	0	0	0 0	0	0 0	0 0	0 0	0 0	0 0	0	0 0
4	3	2	200	2	Ô	1	Ö	Ö	0	ŏ	ŏ	ŏ	Ŏ	ŏ	ő	Ŏ	ő	Ö	ŏ
5	4	1	1110	1	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0
6 7	4 4	2 3	1200 2010	1 2	2 1	0 1	0	1	0 1	0	0	0	0 0	0 0	0 0	0	0 0	0	0 0
8	4	4	3000	3	ō	3	ŏ	ő	ō	1	ő	ő	ő	Õ	ő	ő	0	Õ	Õ
9	5	1	11110	1	1	0	1	0	0	0	1	0	0	0	0	0	0	0	0
10 11	5 5	2	11200 12010	1 1	1 2	0 0	2 1	0 1	0	0	0 0	1 0	0 1	0 0	0 0	0 0	0	0	0 0
12	5	4	13000	1	3	0	0	3	0	Ö	ő	0	Ô	1	Ő	0	Õ	0	0
13	5	5	20110	2	1	1	1	0	1	0	0	0	0	0	1	0	0	0	0
14 15	5 5	6 7	20200 21010	2 2	2 2	1 1	0	1 0	2 2	0 0	0	0	0 0	0 0	0 0	1 0	0	0	0 0
16	5	8	30010	3	1	3	ő	ő	2	1	Ö	Ö	Õ	0	ő	0	Ô	1	Ö
17	5	9	40000	4	0	6	0	0	0	4	0	0	0	0	0	0	0	0	1
18 19	6 6	1 2	111110 111200	1 1	1 1	0 0	1 1	0 0	0 0	0 0	1 2	0	0 0	0 0	0 0	0 0	0	0	0
20	6	3	112010	1	1	0	2	0	0	0	1	1	0	0	0	0	0	0	0
21	6	4	113000	1	1	0	3	0	0	0	0	3	0	0	0	0	0	0	0
22 23	6	5 6	120110 120200	1	2 2	0	1 2	1	0	0	1 0	0	1 2	0	0	0 0	0	0	0
23 24	6 6	7	120200	1 1	2	0	2	1 1	0 0	0 0	0	1 0	2	0 0	0	0	0	0	0 0
25	6	8	130010	1	3	0	1	3	0	0	0	0	2	1	0	0	0	0	0
26 27	6 6	9 10	201110 201200	2 2	1 1	1 1	1 2	0	1	0 0	1 0	0	0 0	0 0	1 2	0	0	0	0 0
28	6	11	201200	2	2	1	1	1	1 2	0	0	1 0	1	0	1	1	0	0	0
29	6	12	203000	2	3	1	0	3	3	0	0	0	0	1	0	3	Õ	0	0
30	6	13	210110	2	2	1	1 0	0	2	0	0	0	0 0	0	1 0	0	1	0	0
31 32	6 6	14 15	210200 300110	2	3 1	1 3	1	1 0	3 2	0 1	0	0	0	0 0	2	1 0	2	0 1	0 0
33	6	16	300200	3	2	3	0	1	4	1	Ŏ	Ö	0	0	0	2	ŏ	2	Ŏ.
34	6	17	301010	3	2	3	0	0	4	1	0	0	0	0	0	0	1	2	0
35 36	6 7	18 1	400010 1111110	4 1	1 1	6 0	0 1	0 0	3 0	4 0	0 1	0 0	0 0	0 0	0 0	0 0	0	3	1 0
37	7	2	1111200	1	i	ŏ	1	ŏ	ŏ	ŏ	1	ŏ	Ö	ő	ő	Õ	Õ	0	ŏ
38	7	3	1112010	1	1	0	1	0	0	0	2	0	0	0	0	0	0	0	0
39 40	7 7	4 5	1113000 1120110	1 1	1 1	0	1 2	0	0	0	3 1	0 1	0 0	0 0	0 0	0	0 0	0 0	0 0
41	7	6	1120200	î	î	ŏ	2	ŏ	ő	ŏ	2	1	ő	ŏ	ő	Õ	ő	Õ	ő
42	7	7	1121010	1	1	0	2	0	0	0	2	1	0	0	0	0	0	0	0
43 44	7 7	8 9	1130010 1201110	1 1	1 2	0	3 1	0	0	0	1	3 0	0 1	0 0	0 0	0 0	0	0	0
45	7	10	1201110	1	2	ő	1	1	ő	ŏ	2	ő	1	0	ő	Ö	0	0	Ő
46	7	11	1202010	1	2	0	2	1	0	0	1	1	2	0	0	0	0	0	0
47 48	7 7	12 13	1203000 1210110	1 1	2 2	0 0	3 2	1 1	0 0	0 0	0 1	3 0	3 2	0 0	0 0	0 0	0	0	0 0
49	7	14	1210200	1	2	ő	3	1	ő	ő	Ô	1	3	0	0	0	0	0	0
50	7	15	1300110	1	3	0	1	3	0	0	1	0	2	1	0	0	0	0	0
51 52	7 7	16 17	1300200 1301010	1 1	3 3	0 0	2 2	3 3	0 0	0	0 0	1 0	4 4	1 1	0 0	0 0	0	0	0 0
53	7	18	2011110	2	1	1	1	0	1	0	1	0	0	0	1	0	0	0	0
54	7	19	2011200	2	1	1	1	0	1	0	2	0	0	0	1	0	0	0	0
55 56	7 7	20 21	2012010 2013000	2 2	1 1	1 1	2	0	1 1	0 0	1 0	1	0 0	0 0	2 3	0 0	0 0	0 0	0 0
57	7	22	2013000	2	2	1	1	1	2	0	1	0	1	0	1	1	0	0	0
58	7	23	2020200	2	2	1	2	1	2	0	0	1	2	0	2	1	0	0	0
59 60	7 7	24 25	2021010 2030010	2 2	2	1 1	2 1	1 3	2	0 0	0 0	0 0	2 2	0 1	2 1	1 3	0	0	0
61	7	26	2101110	2	2	1	1	ō	2	Ö	1	0	0	0	1	0	1	0	0
62	7	27	2101200	2	2	1	2	0	2	0	0	1	0	0	2	0	1	0	0
63 64	7 7	28 29	2102010 2103000	2 2	3 4	1 1	1 0	1 3	3 4	0	0	0	1 0	0 1	1 0	1 3	2	0	0 0
65	7	30	2110110	2	2	1	2	0	2	0	0	0	0	0	2	0	1	0	0
66	7	31	2110200	2	3	1	1	1	3	0	0	0	0	0	1	1	2	0	0
67 68	7 7	32 33	2200200 3001110	2 3	4 1	1 3	0 1	2 0	4 2	0 1	0 1	0 0	0 0	0 0	0 2	2 0	4 0	0 1	0
69	7	34	3001200	3	1	3	2	0	2	1	0	1	0	0	4	0	0	1	0
70	7	35	3002010	3	2	3	1	1	4	1	0	0	1	0	2	2	0	2	0
71 72	7 7	36 37	3003000 3010110	3 3	3 2	3 3	0 1	3 0	6 4	1 1	0	0 0	0 0	1 0	0 2	6 0	0 1	3 2	0 0
73	7	38	3010200	3	3	3	ō	1	6	î	ő	ŏ	ő	ő	0	2	2	3	ŏ

Table 2 (Continued)

embedding frequencies																			
no.	N	no.a	code	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
74	7	39	3101010	3	3	3	0	0	6	1	0	0	0	0	0	0	3	3	0
75	7	40	4000110	4	1	6	1	0	3	4	0	0	0	0	3	0	0	3	1
76 77	7 7	41 42	4000200 4001010	4 4	2 2	6 6	0 0	1 0	6 6	4 4	0	0 0	0	0	0 0	3 0	0 1	6 6	1 1
78	8	1	111111110	1	1	0	1	ő	0	0	1	0	ő	0	0	0	0	0	Ô
79	8	2	11111200	1	1	Ö	1	Ŏ	Ŏ	Ō	1	Õ	Ö	Ö	ō	0	ŏ	Ö	Ō
80	8	3	11112010	1	1	0	1	0	0	0	1	0	0	0	0	0	0	0	0
81	8	4	11113000	1	1	0	1	0	0	0	1	0	0	0	0	0	0	0	0
82 83	8 8	5	11120110 11120200	1	1 1	0	1 1	0	0	0 0	2 2	0 0	0 0	0	0 0	0	0	0 0	0
84	8	6 7	11121210	1	1	0	1	0	0	0	2	0	0	0	0	0	0	0	0
85	8	8	11130010	1	î	ŏ	î	ŏ	ŏ	ő	3	ő	ŏ	ŏ	ŏ	ő	ŏ	ŏ	ŏ
86	8	9	11201110	1	1	0	2	0	0	0	1	1	0	0	0	0	0	0	0
87	8	10	11201200	1	1	0	2	0	0	0	1	1	0	0	0	0	0	0	0
88	8	11	11202010	1	1	0	2	0	0	0	2	1	0	0	0	0	0	0	0
89 90	8 8	12 13	11203000 11210110	1 1	1 1	0	2 2	0	0	0 0	3 2	1 1	0	0	0	0	0	0	0
91	8	13	11210110	1	1	0	2	0	0	0	3	1	0	0	0	0	0	0	0
92	8	15	11300110	î	î	ŏ	3	ŏ	ŏ	ŏ	1	3	ŏ	ŏ	ŏ	ŏ	ŏ	ŏ	ŏ
93	8	16	11300200	1	1	0	3	0	0	0	2	3	0	0	0	0	0	0	0
94	8	17	11301010	1	1	0	3	0	0	0	2	3	0	0	0	0	0	0	0
95	8	18	12011110	1	2	0	1	1	0	0	1	0	1	0	0	0	0	0	0
96 97	8 8	19 20	12011200 12012010	1 1	2 2	0	1 1	1 1	0	0	1 2	0	1 1	0 0	0 0	0 0	0	0 0	0 0
98	8	21	12012010	1	2	ő	1	1	ő	ő	3	0	1	ő	ő	ő	ő	ő	ŏ
99	8	22	12020110	1	2	ŏ	2	1	Õ	Õ	1	1	2	Ö	Ŏ	Ō	Ö	ō	Ō
100	8	23	12020200	1	2	0	2	1	0	0	2	1	2	0	0	0	0	0	0
101	8	24	12021010	1	2	0	2	1	0	0	2	1	2	0	0	0	0	0	0
102	8	25	12030010	1	2	0	3	1	0	0 0	1	3 0	3	0	0	0 0	0	0 0	0
103 104	8 8	26 27	12101110 12101200	1	2 2	0	2 2	1 1	0	0	1 2	0	2 2	0	0	0	0	0	0
105	8	28	12101200	1	2	0	3	1	0	ő	1	1	3	Ö	ő	0	ő	ő	ő
106	8	29	12103000	1	2	0	4	1	0	0	0	3	4	0	0	0	0	0	0
107	8	30	12110110	1	2	0	2	1	0	0	2	0	2	0	0	0	0	0	0
108	8	31	12110200	1	2	0	3	1	0	0	1	1	3	0	0	0	0	0	0
109 110	8 8	32 33	12200200 13001110	1	2 3	0	4 1	1 3	0 0	0 0	0 1	2 0	4 2	0 1	0	0	0	0 0	0
111	8	34	13001110	1	3	0	1	3	0	ő	2	0	2	1	0	0	0	ő	0
112	8	35	13002010	1	3	0	2	3	0	0	1	1	4	1	0	0	0	0	0
113	8	36	13003000	1	3	0	3	3	0	0	0	3	6	1	0	0	0	0	0
114	8	37	13010110	1	3	0	2	3	0	0	1	0	4	1	0	0	0	0	0
115	8	38 39	13010200	1 1	3	0 0	3	3 3	0	0	0 0	0	6 6	1	0 0	0 0	0	0 0	0
116 117	8 8	39 40	13101010 20111110	2	1	1	1	0	1	0	1	0	0	0	1	0	0	0	0
118	8	41	20111100	2	i	1	î	ŏ	1	ő	1	ŏ	ŏ	ő	î	ŏ	ŏ	ő	0
119	8	42	20112010	2	1	1	1	0	1	0	2	0	0	0	1	0	0	0	0
120	8	43	20113000	2	1	1	1	0	1	0	3	0	0	0	1	0	0	0	0
121	8	44	20120110	2	1	1	2	0	1	0	1	1	0	0	2	0	0	0	0
122 123	8 8	45 46	20120200 20121010	2 2	1 1	1 1	2 2	0	1 1	0	2 2	1 1	0 0	0 0	2 2	0	0	0	0
123	8	47	20130010	2	1	1	3	ő	i	ŏ	1	3	ő	ŏ	3	ŏ	ŏ	ŏ	ő
125	8	48	20201110	2	2	1	1	1	2	0	1	0	1	0	1	1	0	0	0
126	8	49	20201200	2	2	1	1	1	2	0	2	0	1	0	1	1	0	0	0
127	8	50	20202010	2	2	1	2	1	2	0	1	1	2	0	2	1	0	0	0
128 129	8 8	51 52	20203000 20210110	2 2	2 2	1 1	3 2	1 1	2 2	0	0 1	3 0	3 2	0 0	3 2	1 1	0	0	0
130	8	53	20210200	2	2	1	3	1	2	ŏ	ō	1	3	Ö	3	i	ő	ŏ	ő
131	8	54	20300110	2	3	1	1	3	3	ō	1	0	2	1	1	3	0	0	0
132	8	55	20300200	2	3	1	2	3	3	0	0	1	4	1	2	3	0	0	0
133	8	56	20301010	2	3	1	2	3	3	0	0	0	4	1	2	3	0	0 0	0
134 135	8 8	57 58	21011110 21011200	2 2	2 2	1 1	1 1	0 0	2 2	0	1 2	0	0 0	0 0	1 1	0	1 1	0	0
136	8	59	21012010	2	2	1	2	ő	2	ŏ	1	1	ŏ	Ö	2	Õ	î	ŏ	ŏ
137	8	60	21013000	2	2	1	3	Ŏ	2	0	ō	3	0	0	3	0	1	0	0
138	8	61	21020110	2	3	1	1	1	3	0	1	0	1	0	1	1	2	0	0
139	8	62	21020200	2	3	1	2	1	3	0	0	1 0	2 2	0 0	2 2	1 1	2 2	0	0
140 141	8 8	63 64	21021010 21030010	2 2	3 4	1 1	2 1	1 3	3 4	0	0 0	0	2	1	1	3	3	0	0
142	8	65	21101110	2	2	1	2	0	2	0	1	Ö	0	0	2	0	1	0	ő
143	8	66	21101200	2	2	1	3	0	2	0	0	1	0	0	3	0	1	0	0
144	8	67	21102010	2	3	1	2	1	3	0	0	0	1	0	2	1	2	0	0
145	8 8	68 69	21103000	2 2	4	1 1	1 1	3 1	4	0	0 1	0	0	1 0	1 1	3 1	3 2	0	0
146	ō	69	22001110	2	3	1	1	1	3	U	1	U	U	U	1	1	2	U	U

Table 2 (Continued)

				embedding frequencies															
no.	N	no.a	code	2	3	4	5	6	7_	8	9	10	11	12	13	14	15	16	17
147	8	70	22001200	2	3	1	2	1	3	0	0	1	0	0	2	1	2	0	0
148	8	71	22002010	2	4	1	1	2	4	0	0	0	1	0	1	2	4	0	0
149	8	72	22003000	2	5	1	0	4	5	0	0	0	0	1	0	4	6	0	0
150	8	73	30011110	3	1	3	1	0	2	1	1	0	0	0	2	0	0	1	0
151	8	74	30011200	3	1	3	1	0	2	1	2	0	0	0	2	0	0	1	0
152	8	75	30012010	3	1	3	2	0	2	1	1	1	0	0	4	0	0	1	0
153	8	76	30013000	3	1	3	3	0	2	1	0	3	0	0	6	0	0	1	0
154	8	77	30020110	3	2	3	1	1	4	1	1	0	1	0	2	2	0	2	0
155	8	78	30020200	3	2	3	2	1	4	1	0	1	2	0	4	2	0	2	0
156	8	79	30021010	3	2	3	2	1	4	1	0	0	2	0	4	2	0	2	0
157	8	80	30030010	3	3	3	1	3	6	1	0	0	2	1	2	6	0	3	0
158	8	81	30101110	3	2	3	1	0	4	1	1	0	0	0	2	0	1	2	0
159	8	82	30101200	3	2	3	2	0	4	1	0	1	0	0	4	0	1	2	0
160	8	83	30102010	3	3	3	1	1	6	1	0	0	1	0	2	2	2	3	0
161	8	84	30103000	3	4	3	0	3	8	1	0	0	0	1	0	6	3	4	0
162	8	85	30110110	3	2	3	2	0	4	1	0	0	0	0	4	0	1	2	0
163	8	86	30110200	3	3	3	1	1	6	1	0	0	0	0	2	2	2	3	0
164	8	87	30200200	3	4	3	0	2	8	1	0	0	0	0	0	4	4	4	0
165	8	88	31010110	3	3	3	1	0	6	1	0	0	0	0	2	0	3	3	0
166	8	89	31010200	3	4	3	0	1	8	1	0	0	0	0	0	2	5	4	0
167	8	90	40001110	4	1	6	1	0	3	4	1	0	0	0	3	0	0	3	1
168	8	91	40001200	4	1	6	2	0	3	4	0	1	0	0	6	0	0	3	1
169	8	92	40002010	4	2	6	1	1	6	4	0	0	1	0	3	3	0	6	1
170	8	93	40003000	4	3	6	0	3	9	4	0	0	0	1	0	9	0	9	1
171	8	94	40010110	4	2	6	1	0	6	4	0	0	0	0	3	0	1	6	1
172	8	95	40010200	4	3	6	0	1	9	4	0	0	0	0	0	3	2	9	1
173	8	96	40101010	4	3	6	0	0	9	4	0	0	0	0	0	0	3	9	1

<sup>&</sup>lt;sup>a</sup> Serial number of rooted trees with fixed number of vertices (see second column).

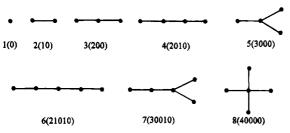


Figure 5. All possible eight subtrees through five vertices. In Table 1 are given embedding frequencies that correspond to these subtrees.

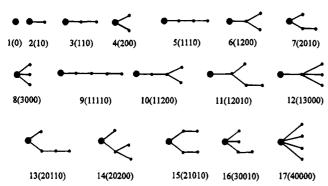


Figure 6. All possible rooted subtrees through five vertices. In Table 2 are given only embedding frequencies that correspond to rooted subtrees labeled by 2-17, whereas the first rooted subtree composed of one vertex (root) is not considered, its embedding frequency being automatically equal to one for any rooted tree.

#### DISCUSSION

The embedding frequencies are very useful graph-theoretical descriptors of molecular graphs for construction of structure-activity and/or structure-property relationships. They reflect in a natural way, closely related to a thinking of chemists, structural features of molecular graphs. Their

calculation can be simply done for acyclic molecular graphs mainly due to (i) the possibility to detect isomorphism between trees by Read's linear codes and (ii) the fact that for trees each subtree is automatically induced by a vertex subset. A simple pruning procedure for construction of embedding frequencies of trees as well as rooted trees is described in section 2. It can be considerably accelerated by making use of conditions (6a,b) detecting on the basis of valence vectors whether a smaller tree can be a subtree of a larger tree. If one of the conditions is not satisfied, then the branch of search algorithm is stopped and the method returns to the previous branching point of the search tree. The calculated embedding frequencies of trees and rooted trees are listed in Tables 1 and 2, respectively.

The present method of calculation of embedding frequencies may be simply generalized for general acyclic molecular graphs (i.e., which contain also double and triple bonds and heteroatoms).<sup>19</sup> For instance, if we would like to calculate embedding frequencies of alkynes, then the edges of (rooted) trees should also be specified by the so-called bond multiplicities. Read's linear codes are simply generalized for trees with multiple edges, so that each entry (except of the first entry) should be enlarged by an additional entry (integer), which specifies the multiplicity of the edge; for details see ref 19.

The embedding-frequency approach has been recently successfully used in our papers dedicated to neural network applications to predict some thermochemical properties of alkanes<sup>20,21</sup> and also to classify inductive and resonance effects of functional groups.<sup>22</sup> Recently, similar applications are under way for a broad classes of acyclic molecules with heteroatoms.<sup>23</sup> Our results indicate that neural networks based on the embedding-frequency descriptors provide relationships that are comparable (or even better) than other results obtained by making use of other topological indices as descriptors. <sup>24–26</sup> Neural network predictions of <sup>13</sup>C-NMR chemical shifts done by one (V.K.) of the present authors <sup>27,28</sup> were based on descriptors that are closely related to the method of embedding frequencies of rooted trees. Currently, we are repeating these calculations in the present framework, and the preliminary results are very promising.

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