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STATISTICS OF EQUISEPARABLE TREES AND CHEMICAL TREES

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Abstract

If T is a tree and e its edge, then $T - e$ consists of two components, with $n_1(e|T)$ and $n_2(e|T)$ vertices. Conventionally, $n_1(e|T) \leq n_2(e|T)$. If T' and T'' are two trees of the same order n, and if their edges $e'_1, e'_2, \ldots, e'_{n-1}$ and $e''_1, e''_2, \ldots, e''_{n-1}$ can be labeled so that $n_1(e'_i|T') = n_1(e''_i|T'')$ holds for all $i = 1, 2, \ldots, n-1$, then T' and T'' are said to be equiseparable. We examined n-vertex trees and chemical trees ($7 \leq n \leq 20$) with regard to equiseparability. There exist very large families of equiseparable trees and chemical trees, and only a relatively few of them have no equiseparable mate.

Let T be a tree and $e = (xy)$ be its edge. By $n_1(e|T)$ and $n_2(e|T)$ we denote the number of vertices of T, lying closer to vertex x than to vertex y, and closer to vertex y than to vertex x, respectively, i. e.,

$$\begin{aligned} n_1(e|T) &= |\{u \in V(T)\,;\, d(u,x) < d(v,x)\}| \\ n_2(e|T) &= |\{u \in V(T)\,;\, d(u,x) > d(v,x)\}| \,. \end{aligned}$$

In other words, the subgraph $T - e$, obtained by deleting the edge e from T, consists of two components, with $n_1(e|T)$ and $n_2(e|T)$ vertices. Conventionally, $n_1(e|T) \leq n_2(e|T)$.

The quantities $n_1(e|T)$ and $n_2(e|T)$ are encountered already in the seminal paper [1], where the formula

$$W(T) = \sum_e n_1(e|T) \cdot n_2(e|T) \tag{1}$$

is put forward for the calculation of (what nowadays is called) the Wiener index W. For the further development of the research based on Eq. (1) see the reviews [2, 3].

Few years ago Eq. (1) served as a motivation for the introduction of the *modified Wiener index* [4]

$$^{m}W(T) = \sum_e [n_1(e|T) \cdot n_2(e|T)]^{-1} \tag{2}$$

and, more recently, the *variable Wiener index* [5–9]

$$W_\lambda(T) = \sum_e [n_1(e|T) \cdot n_2(e|T)]^\lambda \tag{3}$$

with λ being an adjustable real number. Of course, for $\lambda = +1$ and $\lambda = -1$, the variable Wiener index reduces, respectively, to the ordinary and to the modified Wiener index.

Another structure-descriptor U, proposed by Zenkevich, can be expressed in terms of the numbers $n_1(e|T)$ and $n_2(e|T)$ [10–12]:

$$U(T) = \sum_e \sqrt{\frac{(C+2H)n + 2H}{[(C+2H)n_1(e|T) + H]\,[(C+2H)n_2(e|T) + H]}} \tag{4}$$

where $C \approx 12.0$ and $H \approx 1.0$ are the relative atomic masses of carbon and hydrogen, respectively.

In Eqs. (1)–(4) the summation goes over all edges of the tree T.

Studies of the above mentioned structure-descriptors lead us to the concept of *equiseparable trees* [13]. Two trees T' and T'' of equal order n are said to be equiseparable if their edges $e'_1, e'_2, \ldots, e'_{n-1}$ and $e''_1, e''_2, \ldots, e''_{n-1}$ can be labeled so that the equality $n_1(e'_i|T') = n_1(e''_i|T'')$ holds for all $i = 1, 2, \ldots, n-1$. Equiseparable trees necessarily have equal W_λ-values (for all λ) as well equal Zenkevich indices U. Consequently, the molecules represented by equiseparable chemical trees are expected to have many similar physico-chemical features.

General procedures for constructing pairs of equiseparable trees were developed [13, 14], and it gradually became evident that equiseparable trees and chemical trees occur in large families. Furthermore, equiseparability happens to be a wide-spread phenomenon and trees having no equiseparable mate are relatively rare.

In order to gain more information of the occurrence of equiseparable trees, we performed a systematic study of all trees and chemical trees with $n \leq 20$ vertices.

The main results obtained are presented in Tables 1 & 2 (for trees) and Tables 3 & 4 (for chemical trees). Additional data can be obtained from the authors.

From Tables 1–4 we see that there exist very large families of equiseparable trees and chemical trees, and that only a relatively small number of them have no equiseparable mate. In Fig. 1 is shown that with the increasing number of vertices, the number of trees without an equiseparable mate becomes much smaller than the total number of trees.

F	$n = 7$	$n = 8$	$n = 9$	$n = 10$	$n = 11$	$n = 12$	$n = 13$
1	9	17	22	47	57	106	147
2	1	3	9	18	35	73	108
3	–	–	1	3	9	20	50
4	–	–	1	1	7	12	34
5	–	–	–	2	6	16	23
F	$n = 14$	$n = 15$	$n = 16$	$n = 17$	$n = 18$	$n = 19$	$n = 20$
1	275	316	670	805	1539	1923	3695
2	215	329	625	892	1752	2466	4783
3	98	149	339	501	961	1385	2747
4	66	136	259	466	896	1508	2904
5	62	97	205	309	688	940	1896

Table 1. Number of families of equiseparable n-vertex trees of small size (F). The case $F = 1$ pertains to trees having no equiseparable mate.

n					
7	2	1	1	1	1
8	2	2	2	1	1
9	4	3	2	2	2
10	5	5	4	3	3
11	9	8	6	5	5
12	12	11	9	8	8
13	20	20	17	16	15
14	34	27	25	23	22
15	54	47	45	44	40
16	84	70	70	67	63
17	138	135	126	109	108
18	227	206	198	196	177
19	370	365	330	328	317
20	603	597	564	563	543

Table 2. Sizes of the five largest families of equiseparable n-vertex trees.

F	$n = 7$	$n = 8$	$n = 9$	$n = 10$	$n = 11$	$n = 12$	$n = 13$
1	7	14	19	44	54	105	145
2	1	2	5	6	20	39	81
3	–	–	2	5	9	22	37
4	–	–	–	1	5	11	23
5	–	–	–	–	1	2	9
F	$n = 14$	$n = 15$	$n = 16$	$n = 17$	$n = 18$	$n = 19$	$n = 20$
1	287	347	768	943	1876	2396	4783
2	157	269	502	823	1653	2495	4991
3	75	126	285	439	861	1347	2727
4	52	97	218	377	777	1393	2689
5	28	64	123	235	488	723	1542

Table 3. Number of families of equiseparable n-vertex chemical trees of small size (F). The case $F = 1$ pertains to chemical trees having no equiseparable mate.

n					
7	2	1	1	1	1
8	2	2	1	1	1
9	3	3	2	2	2
10	4	3	3	3	3
11	7	6	5	4	4
12	8	7	7	6	6
13	15	11	11	11	11
14	20	20	18	15	14
15	35	31	27	27	25
16	49	42	40	40	37
17	80	75	69	68	67
18	123	116	112	104	93
19	203	181	180	170	162
20	314	295	291	286	252

Table 4. Sizes of the five largest families of equiseparable n-vertex chemical trees.

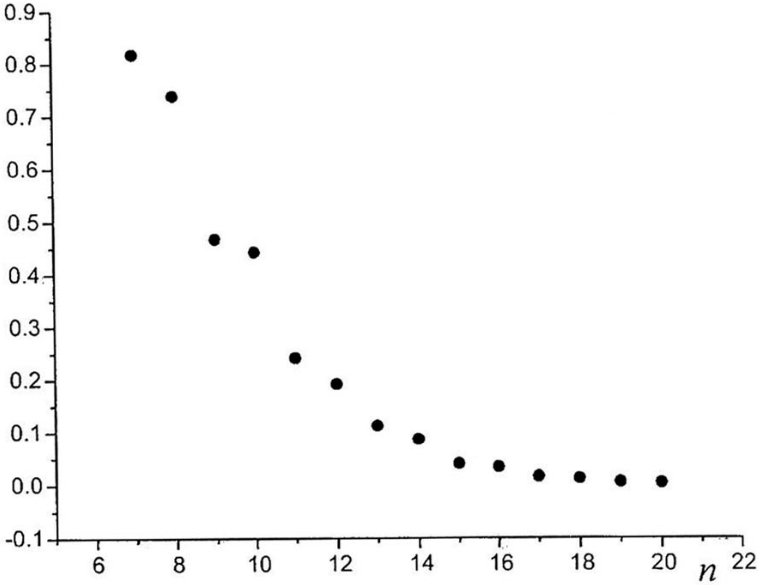

Fig. 1. The ratio between the number of n-vertex trees without an equiseparable mate and the total number of n-vertex trees.

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