NONISOMORPHIC GRAPHS WITH IDENTICAL ATOMIC COUNTS OF SELF-RETURNING WALKS: ISOCODAL GRAPHS

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Abstract

On the basis of endospectral graphs, we present a graphical method for obtaining pairs of nonisomorphic graphs with identical atomic counts of self-returning walks.

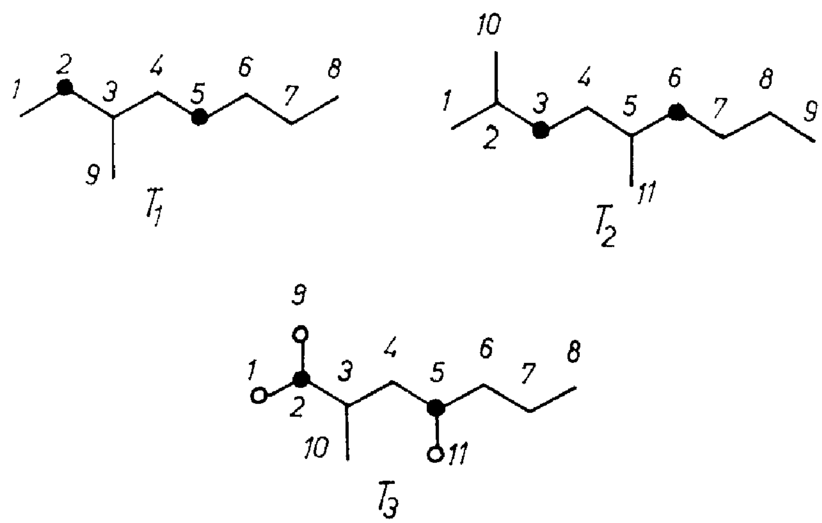
1. Introduction

Chemical graph theory has attracted an increasing research interest in recent years [1–7]. Among the large variety of topics treated, the graph isomorphism problem has received considerable attention. One way of approaching this problem is to search for a set of graph invariants and then to test the selectivity of the selected set of graph invariants over an extensive set of graphs. If some pairs of nonisomorphic graphs are found to have the same set of graph invariants, it is important to study under what structural conditions such a degeneracy appears as well as the methods to avoid it. If no pairs of nonisomorphic graphs with degenerate sets of graph invariants are found, the selected set of invariants may be recommended for further use, albeit with no guarantee that it will always distinguish some untested nonisomorphic graphs. Among the large class of graph invariants, we mention here graph theoretic polynomials, spectral moments, and topological indices.

Although it was initially conjectured that the characteristic polynomial and its spectrum might be used as unique descriptors of graphs, nonisomorphic graphs with the same characteristic polynomial were found [8–14], and called isospectral or cospectral graphs.

Other sets of graph invariants were defined on the basis of self-returning walks [15–17]. A walk in a graph is a sequence of edges which can be continuously traversed, starting from any vertex and ending on any vertex. Repeated use of the same edge or edges is allowed. A self-returning walk is a walk starting and finishing at the same vertex. The length of a walk is the total number of edges that are traversed.

Self-returning walks of length k may be computed by considering the diagonal elements of the first k powers of the adjacency matrix $\mathbf{A}$, due to the fact that each diagonal element $(\mathbf{A}^k)_{ii}$ of the matrix $\mathbf{A}^k$ can be interpreted as the sum of all self-returning walks of length k from/to vertex i. The sequence of integers $\{(\mathbf{A}^1)_{ii}, (\mathbf{A}^2)_{ii}, \ldots, (\mathbf{A}^N)_{ii}\}$ defines the atomic code of the atom i in a molecule. The atomic code characterizes the environment of a given atom in a molecule. Randić [15] conjectured that the atomic codes defined on the basis of self-returning walks are a complete set of graph invariants, i.e. there is no pair of nonisomorphic graphs with the same collection of atomic codes. As examples, the atomic codes of trees T_1, T_2 and T_3 are given in tables 1–3. Only even-length walks are given, because in trees there are no odd-length self-returning walks.



Scheme 1.

Table 1

Atomic codes, structural codes and spectral moments of the tree T_1. In this and subsequent tables, L represents the length of the self-returning walks.

L	Vertex									SM
	1	2	3	4	5	6	7	8	9	
2	1	2	3	2	2	2	2	1	1	16
4	2	6	11	7	6	6	5	2	3	48
6	6	21	42	27	21	19	14	5	11	166
8	21	78	163	107	78	63	42	14	42	608
SC	30	107	219	143	107	90	63	22	57	

Table 2

Atomic codes, structural codes and spectral moments of the tree T_2.

L	Vertex 1	2	3	4	5	6	7	8	9	10	11	SM
2	1	3	2	2	3	2	2	2	1	1	1	20
4	3	10	7	7	11	7	6	5	2	3	3	64
6	10	35	27	28	43	27	20	14	5	10	11	230
8	35	127	107	116	174	107	71	43	14	35	43	872
10	127	475	431	487	718	431	264	143	43	127	174	3420
SC	176	650	574	640	949	574	363	207	65	176	232	

Table 3

Atomic codes, structural codes and spectral moments of the tree T_3.

L	Vertex 1	2	3	4	5	6	7	8	9	10	11	SM
2	1	3	3	2	3	2	2	1	1	1	1	20
4	3	11	12	8	11	7	5	2	3	3	3	68
6	11	44	52	35	44	26	15	5	11	12	11	266
8	44	184	231	158	184	101	51	15	44	52	44	1108
10	184	791	1038	721	791	407	188	51	184	231	184	4770
SC	243	1033	1336	924	1033	543	261	74	243	299	243	

However, in certain cases, the atomic code of individual atoms in a molecule is not unique. An example of such a case is vertices 2 and 5 of tree T_1.

The spectral moment (SM) of order k is obtained by summing all diagonal elements of $(\mathbf{A}^k)$ and corresponds to the count of all self-returning walks of length k for the given molecule. The sequences of spectral moments for trees T_1, T_2 and T_3 are given in tables 1, 2 and 3, respectively.

The structural code of atom i (SC_i) was defined as [16,17]

$$\mathrm{SC}_i = \sum_{k=1}^{N} (\mathbf{A}^k)_{ii}. \tag{1}$$

Based on the SC, Barysz and Trinajstić [16,17] defined the ordered structural code (OSC) as the ascending ordered sequence of SCs in a molecule. For the tree T_1, the OSC sequence is

$$\mathrm{OSC}(T_1) = \{22, 30, 57, 63, 90, 107, 107, 143, 219\}.$$

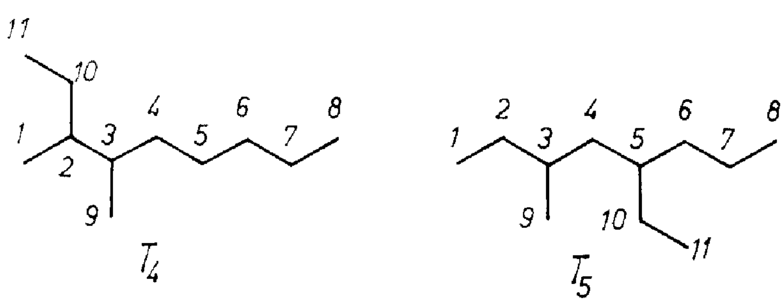
On the basis of the OSC, Barysz and Trinajstić proposed the following conjecture: Two trees are isomorphic if and only if they have identical ordered structural codes.

We will offer counterexamples to the conjectures proposed by Randić [15] and by Barysz and Trinajstić [16], and we will give a structural condition for two nonisomorphic graphs to present the same set of atomic codes.

2. Isocodal graphs

The concept of endospectral trees appeared in connection with the problem of isospectral trees [18–21]. An endospectral tree is a tree with a pair (or several sets) of topologically distinct vertices having identical atomic codes. For example, tree T_1 has two endospectral vertices, namely 2 and 5; any subgraph attached to either vertex 2 or vertex 5 produces a pair of isospectral graphs. Tree T_2 has a pair of endospectral vertices represented by vertices 3 and 6, and tree T_3 has two sets of endospectral vertices: 1, 9 and 11; 2 and 5. The endospectral vertices are depicted as distinct circles. Recently, the collection of endospectral trees up to 16 vertices was reported [22].

A pair of endospectral vertices in a graph exhibits a remarkable property: if we connect a subgraph to any of the endospectral vertices, then vertices belonging to this subgraph will have identical atomic codes, irrespective of the site of connection.



Scheme 2.

Table 4

Atomic codes, structural codes and spectral moments of the tree T_4.

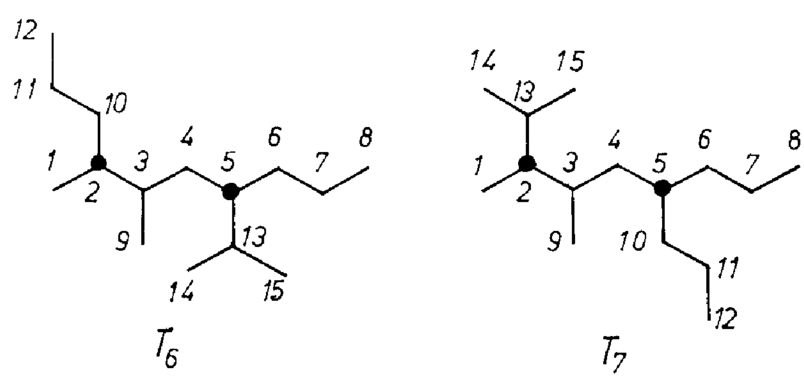
L	Vertex 1	2	3	4	5	6	7	8	9	10	11	SM
2	1	3	3	2	2	2	2	1	1	2	1	20
4	3	12	12	7	6	6	5	2	3	6	2	64
6	12	51	52	28	21	19	14	5	12	22	6	242
8	51	222	231	119	79	63	42	14	52	89	22	984
10	222	979	1035	520	312	219	133	42	231	378	89	4160
SC	289	1267	1333	676	420	309	196	64	299	497	120	

Table 5

Atomic codes, structural codes and spectral moments of the tree T_5.

L	Vertex 1	2	3	4	5	6	7	8	9	10	11	SM
2	1	2	3	2	3	2	2	1	1	2	1	20
4	2	6	11	8	12	7	5	2	3	6	2	64
6	6	21	43	35	51	27	15	5	11	22	6	242
8	21	79	175	156	222	110	52	15	43	89	22	984
10	79	312	734	699	979	464	199	52	175	378	89	4160
SC	109	420	966	900	1267	610	273	75	233	497	120	

For example, trees T_4 and T_5 are obtained on the basis of the endospectral tree T_1 by inserting a subgraph representing the ethyl group to vertex 2 or 5, respectively. The atomic codes, spectral moments and structural codes of T_4 and T_5 are given in tables 4 and 5. As is easily observed, vertices 10 and 11 from trees T_4 and T_5, belonging to the attached subgraph, exhibit identical atomic codes when this subgraph is connected to vertex 2 or 5, respectively. The same fact is observed if we connect to tree T_1 a propyl and an isopropyl group, first to vertices 2 and 5, and then to vertices 5 and 2, obtaining trees T_6 and T_7, respectively, whose atomic codes, spectral moments and structural codes are given in tables 6 and 7. Again, the vertices belonging to the subgraphs have identical atomic codes, irrespective of the endospectral vertex they are bonded to.



Scheme 3.

Based on this finding, we give a method for constructing pairs of nonisomorphic graphs with identical atomic codes:

Table 6

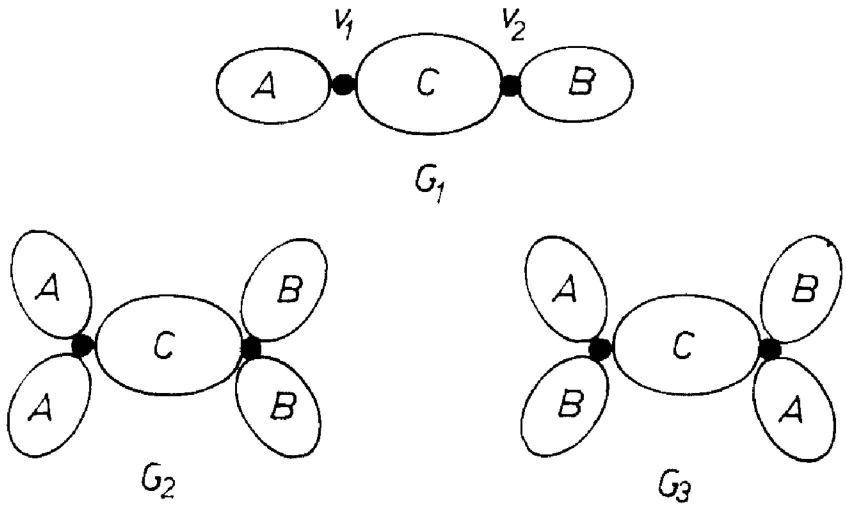
Atomic codes, structural codes and spectral moments of the tree T_6.

L	Vertex 1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	SM
2	1	3	3	2	3	2	2	1	1	2	2	1	3	1	1	28
4	3	12	12	8	13	7	5	2	3	7	5	2	11	3	3	96
6	12	52	53	37	60	28	15	5	12	27	15	5	45	11	11	388
8	52	232	245	179	282	121	53	15	53	111	52	15	196	45	45	1696
10	232	1054	1160	879	1340	547	212	53	245	476	200	52	886	196	196	7728
12	1054	4860	5568	4340	6422	2540	918	212	1160	2102	824	200	4100	886	886	36072
14	4860	22700	26956	21474	30992	11996	4164	918	5568	9488	3550	824	19278	4100	4100	170968
SC	6214	28913	33997	26919	39112	15241	5369	1206	7042	12213	4648	1099	24519	5242	5242	

Table 7

Atomic codes, structural codes and spectral moments of the tree T_7.

L	Vertex 1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	SM
2	1	3	3	2	3	2	2	1	1	2	2	1	3	1	1	28
4	3	13	12	8	12	7	5	2	3	7	5	2	11	3	3	96
6	13	60	54	36	52	27	15	5	12	27	15	5	45	11	11	388
8	60	282	256	170	232	111	52	15	54	111	52	15	196	45	45	1696
10	282	1340	1242	820	1054	476	200	52	256	476	200	52	886	196	196	7728
12	1340	6422	6088	3996	4860	2102	824	200	1242	2102	824	200	4100	886	886	36072
14	6422	30992	29984	19580	22700	9488	3550	824	6088	9488	3550	824	19278	4100	4100	170968
SC	8121	39112	37639	24612	28913	12213	4648	1099	7656	12213	4648	1099	24519	5242	5242	



Scheme 4.

Let G_1 be an endospectral graph having two endospectral vertices V_1 and V_2, and containing a subgraph C which is symmetrical with respect to the vertices V_1 and V_2. We make no assumption on the structure of the subgraphs A and B, with cutpoints to V_1 and V_2, respectively. Graph G_2 is obtained by attaching two subgraphs A to vertex V_1 and two subgraphs B to vertex V_2, while graph G_3 is obtained by attaching a pair of subgraphs A and B to each vertex V_1 and V_2. Obviously, graphs G_2 and G_3 present the same set of atomic codes; such a pair of graphs is called a pair of isocodal graphs. As a consequence, graphs G_2 and G_3 will have identical OSCs.

We will use endospectral trees from the recently reported collection [22] in order to verify the above rule.

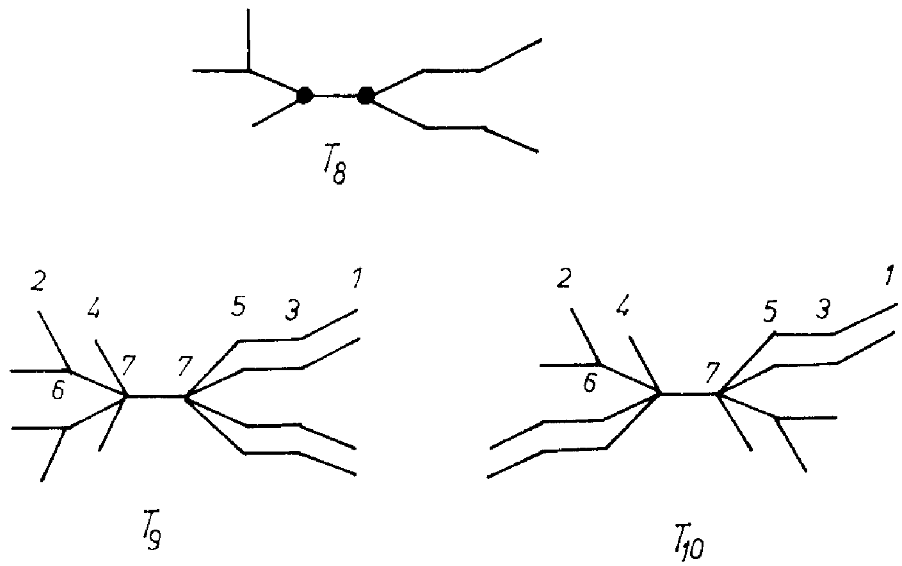
Because it is possible for two or more vertices in a graph to possess the same SC, for the sake of brevity we will note the OSC of a graph G in a more condensed form:

$$\mathrm{OSC}(G) = \{\mathrm{SC}_i^j\}, \qquad i = 1, 2, \ldots, k,$$

where $\mathrm{SC}_i < \mathrm{SC}_{i+1}$, k is the number of distinct values of SCs and j is the number of vertices with the same structural count SC_i. For the same reason, the vertices of a graph will be numbered from 1 to k, and from a set of topologically equivalent vertices exhibiting the same value of SC, the label will be depicted only for one vertex from the whole set.

The simplest situation which fulfills the above conditions is represented by an endospectral tree with adjacent endospectral vertices.

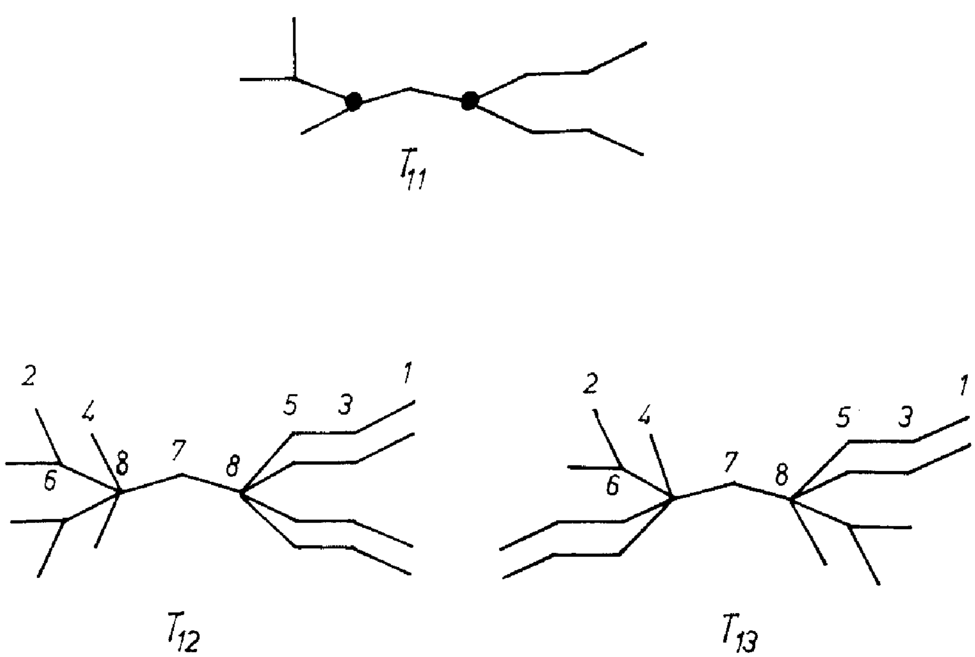
The first endospectral tree suitable for our scope is T_8; it is a 3-tree (its highest vertex degree is 3) with 12 vertices. It gives two isocodal 5-trees with 22 vertices, T_9 and T_{10}, with the following OSC:



Scheme 5.

$$\mathrm{OSC}(T_9) = \mathrm{OSC}(T_{10}) = \{10993968^4,\ 81780585^4,\ 81782632^4,\ 326186175^2,\ 456769535^4,\ 609336737^2,\ 2433610487^2\}.$$

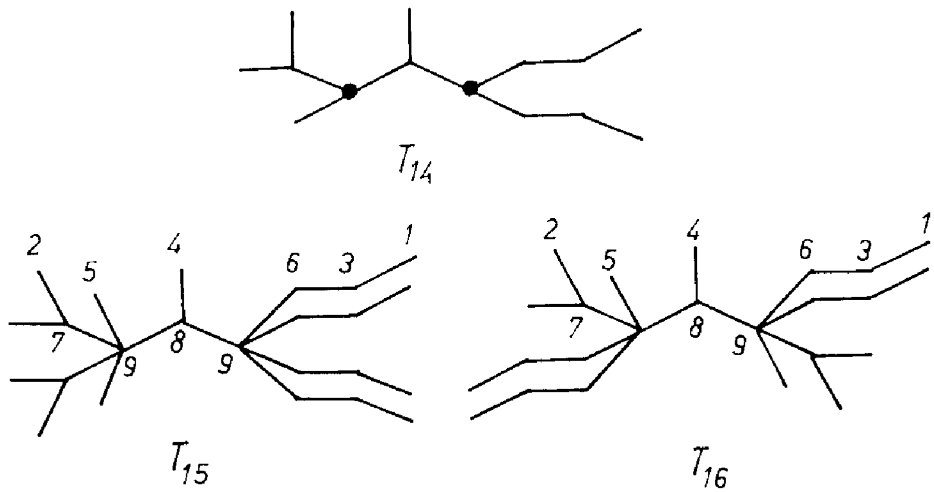
If we insert a vertex between the two endospectral vertices in T_8, we obtain another endospectral tree, namely T_{11}, which gives another pair of isocodal 5-trees with 23 vertices, T_{12} and T_{13}:



Scheme 6.

The common OSC of T_{12} and T_{13} is

$$\mathrm{OSC}(T_{12}) = \mathrm{OSC}(T_{13}) = \{5389823^4,\ 357411834^4,\ 357432304^4,\ 1171261442^2,\ 1724431354^4,\ 2385356782^2,\ 440795134,\ 7887564792^2\}.$$



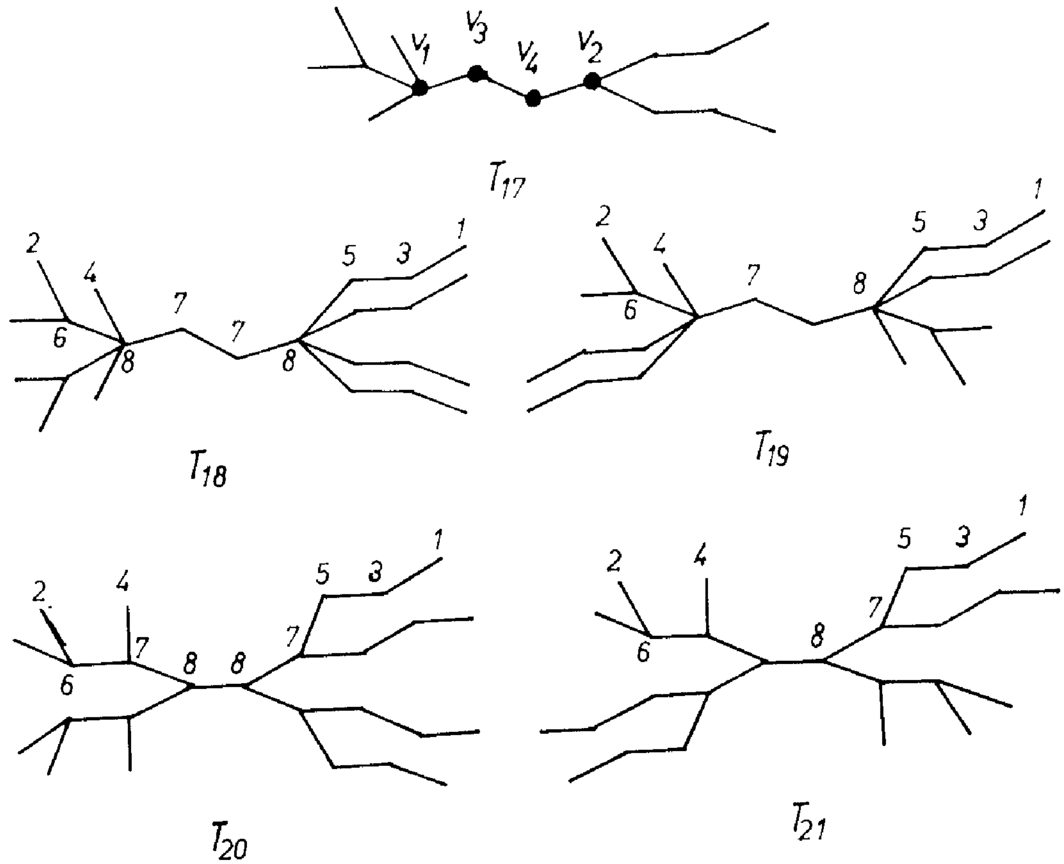
Scheme 7.

By inserting two vertices between the two endospectral vertices in T_8, we obtain either T_{14}, which gives the pair T_{15} and T_{16} of isocodal trees, or T_{17} with two pairs of endospectral vertices: v_1 and v_2, and v_3 and v_4, respectively. The first pair of vertices generates another pair of 5-trees with 24 vertices, namely T_{18} and T_{19}, but the second pair generates a pair of 3-trees with 26 vertices, T_{20} and T_{21}. This is a remarkable fact from an organic chemical viewpoint because the molecular graphs of organic compounds have degrees of at most four (3- or 4-trees in the present case):

$$\mathrm{OSC}(T_{15}) = \mathrm{OSC}(T_{16}) = \{46812829^4, 326332576^4, 326336671^4, 862276952, 1168169390^2, 1680404245^4, 2286256568^2, 6130867808, 8237817040^2\},$$

$$\mathrm{OSC}(T_{18}) = \mathrm{OSC}(T_{19}) = \{28599092^4, 180628629^4, 180632724^4, 536105520^2, 811573692^4, 1144231858^2, 1199921556^2, 3413685996^2\},$$

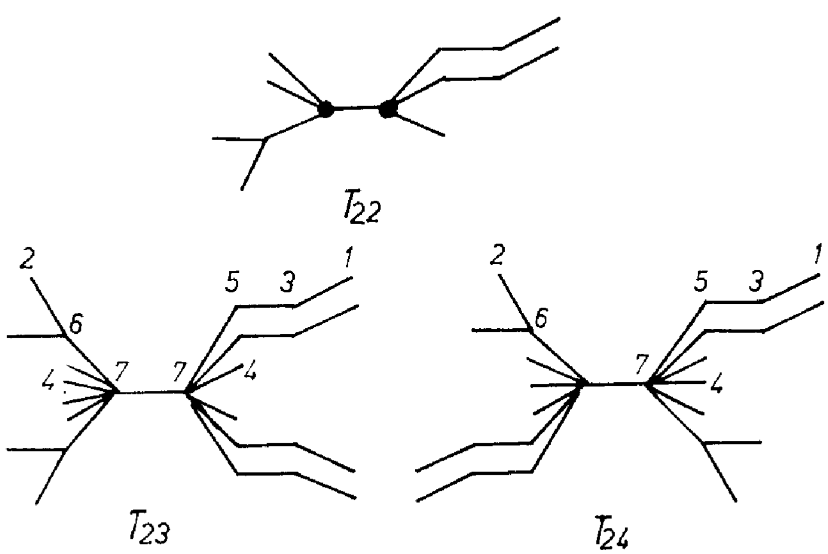
$$\mathrm{OSC}(T_{20}) = \mathrm{OSC}(T_{21}) = \{28888096^4, 166851459^4, 166859650^4, 418773019^2, 665828031^4, 970642853^2, 2458779709^4, 4744617195^2\}.$$



Scheme 8.

Thus, we can generate a whole family of isocodal 4-trees by inserting certain fragments between the two endospectral vertices from T_8. In what follows, we will concentrate on new families of isocodal graphs.

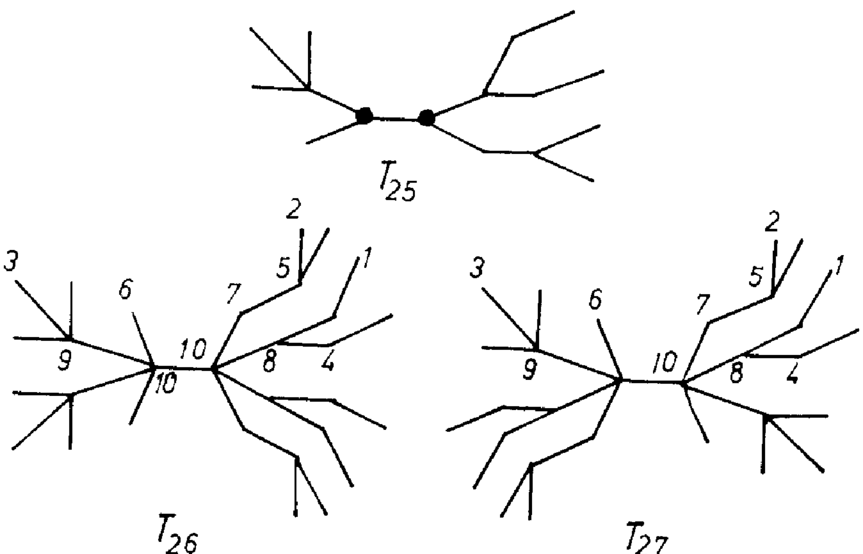
The 4-tree T_{22} with 14 vertices generates a pair of 7-trees with 26 vertices, T_{23} and T_{24}:



Scheme 9.

$$\mathrm{OSC}(T_{23}) = \mathrm{OSC}(T_{24})$$
$$= \{6709799606^4, 64544818777^4, 64544826968^4, 389784576881^6, 498744831999^4, 621124669947^2, 3752054583059^2\}.$$

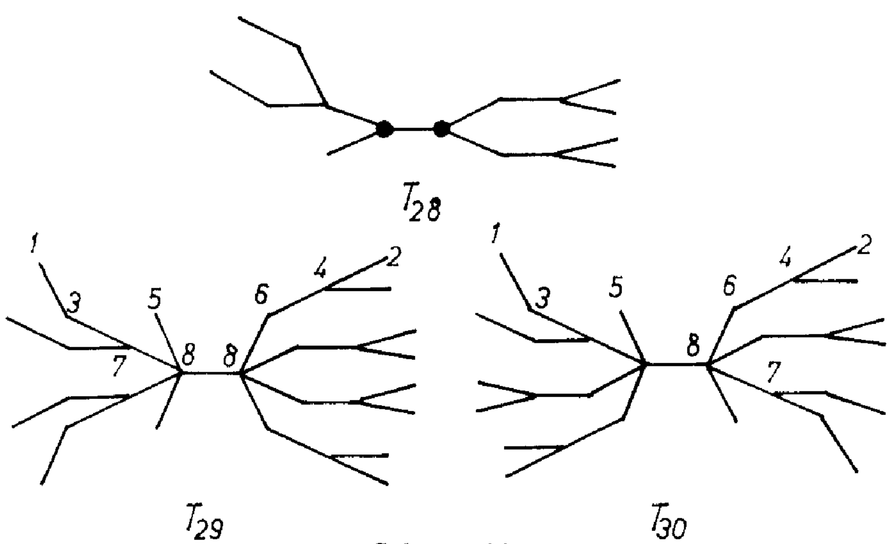
In the collection of endospectral trees [22], we can find another endospectral tree T_{25} with 16 vertices and with adjacent endospectral vertices, being able to produce isocodal trees T_{26} and T_{27}, respectively:



Scheme 10.

$$\mathrm{OSC}(T_{26}) = \mathrm{OSC}(T_{27})$$
$$= \{984743378434^4, 98477925062^4, 789520425955^6, 789524013189^4, 789534774861^2, 2482016653517^2, 3568696577929^2, 4852318003559^2, 6332880930407^2, 19919283678197^2\}.$$

The last endospectral tree from the collection [22] with adjacent endospectral vertices is T_{28}, which generates the isocodal pair of 5-trees represented by T_{29} and T_{30}:

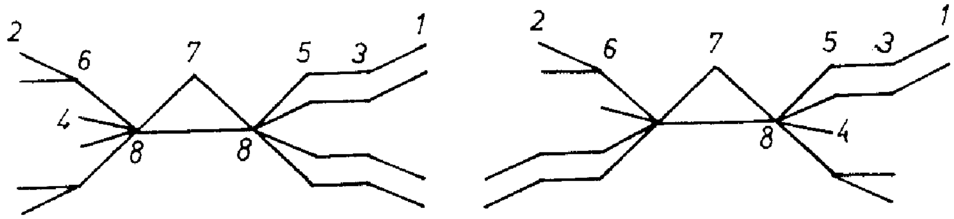


Scheme 11.

$$\begin{aligned}\mathrm{OSC}(T_{29}) &= \mathrm{OSC}(T_{30})\\ &= \{60304839853^4, 60308427072^8, 459460577631^4, 459471339303^4,\\ &\qquad 1287961113515^2, 1905361656761^4, 2643364705245^2, 9821264538247^2\}.\end{aligned}$$

By inserting a linear subgraph between the endospectral vertices from the trees T_{22}, T_{25} and T_{28}, respectively, new families of isocodal 4-trees can be generated.

The method of constructing pairs of isocodal graphs enables one to obtain, on the basis of the mentioned endospectral trees, pairs of isocodal cyclic graphs. The first pair is generated from T_{11} and represents a pair of three-membered cyclic graphs with 23 vertices and maximum degree 6, therefore with no organic chemical counterpart, namely R_1 and R_2:

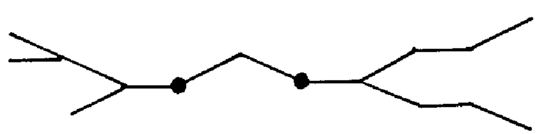


R_1 R_2

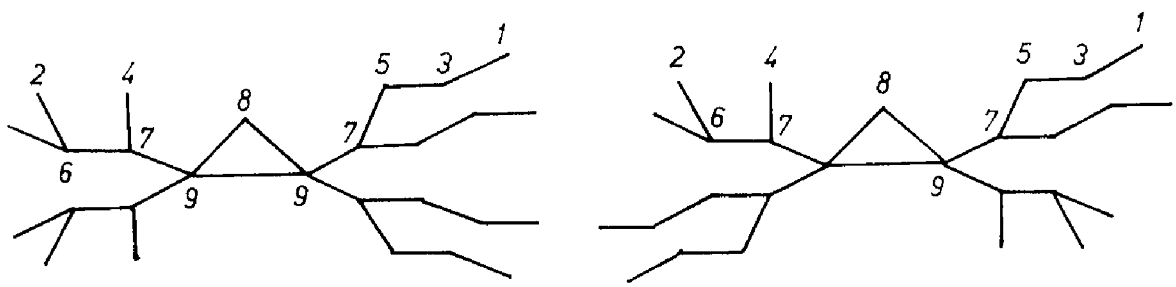
Scheme 12.

$$\begin{aligned}\mathrm{OSC}(R_1) = \mathrm{OSC}(R_2) = \{&5389823^4, 35741183^4, 35743230^4, 117126144^2,\\ &172443135^4, 238535678^2, 440795134, 788756479^2\}.\end{aligned}$$

A pair of isocodal graphs containing three-membered rings with maximum degree 4, R_3 and R_4, can be obtained on the basis of the endospectral tree T_{31}, obtained in turn from the tree T_8:



T_{31}



R_3 R_4

Scheme 13.

$$\mathrm{OSC}(R_3) = \mathrm{OSC}(R_4) = \{21186506^4, 114740394^4, 114748585^4, 251923499^2, 417861151^4, 626155433^2, 1391521642^4, 1491914666, 2231804329^2\}.$$

We have presented a method for obtaining pairs of isocodal graphs, giving counterexamples to two conjectures concerning the problem of graph isomorphism. The smallest pair of isocodal trees is represented by 5-trees with 22 vertices, while the smallest pair of 4-trees is represented by a pair of trees with 26 vertices. Several pairs of isocodal cyclic graphs were also obtained.

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