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ON ISOSPECTRAL BENZENOID GRAPHS

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Abstract

The recently proposed procedure [5] for the construction of isospectral benzenoid graphs has been examined in detail. Necessary and sufficient conditions for the construction of isospectral benzenoid graphs with isomorphic H-graphs are formulated. The inapplicability of the procedure for the construction of isospectral benzenoid graphs with an even number of vertices has been proven.

1. Introduction

Graph isospectrality and related subjects (e.g. endospectrality of vertices) are continuously drawing the attention of researchers in the fields of graph theory and mathematical chemistry [1]. Quite recently, a series of papers reporting new insights has appeared [2–5]. The present paper is a continuation of the study of the isospectrality of benzenoid graphs. The interest in this subject has suddenly been increased after the conjecture on the non-existence of isospectral benzenoid graphs (IBGs) was announced [6]. Shortly after, this conjecture was (partially) disproved by a procedure designed especially for constructing IBGs [5].

The procedure is based on a method proposed by Heilbronner [7] and therefore we call it Heilbronner-like. (A precise definition of the Heilbronner-like procedure is given later in this paper.) In addition to Heilbronner's original method [7], the approach used in [5] points out some rules specific for benzenoid graphs. In this paper, we examine these specific rules in view of their necessity and sufficiency.

So far, by this procedure only IBGs with an odd number of vertices have been generated. Here, we prove that this is an unavoidable limitation of the Heilbronner-like procedure, i.e. that IBGs with an even number of vertices (and, consequently, those with a Kekulé structure) cannot be obtained in this way.

2. Heilbronner-like procedure for the construction of IBGs

A bipartite graph G can be colored with two colors so that no two adjacent vertices have the same color. For a given colored G, an H-graph $H(G)$ is obtained by the following steps: (i) vertices of one chosen color are removed together with incident (i.e. all) edges; (ii) the remaining vertices are reconnected: between each two vertices, one inserts as many edges as they had common neighbors in G; (iii) to each vertex, one adds as many loops as it had neighbors in G. In this way, two (in the general case different) $H(G)$ graphs can be obtained. If the vertices of G are conveniently numbered, the square of its adjacency matrix possesses a block-diagonal form. The two possible $H(G)$ graphs are related to these blocks as to the adjacency matrices [7]. H-graphs with the loops removed will be referred to as H'-graphs.

It has been shown in [7] that two bipartite graphs G_1 and G_2 with an equal number of vertices are isospectral if they possess an isomorphic pair $\{H(G_1), H(G_2)\}$. According to Heilbronner's original procedure, one tries to construct an isospectral pair by starting from a given G_1, and by attempting to reconstruct a different G_2 from $H(G_1)$, so that $H(G_1) \cong H(G_2)$. An illustrative example is depicted in fig. 1. Any other procedure for the construction of isospectral bipartite graphs will be called *Heilbronner-like* if and only if the isospectrality of the constructed graphs is implied by the isomorphism of their H-graphs.

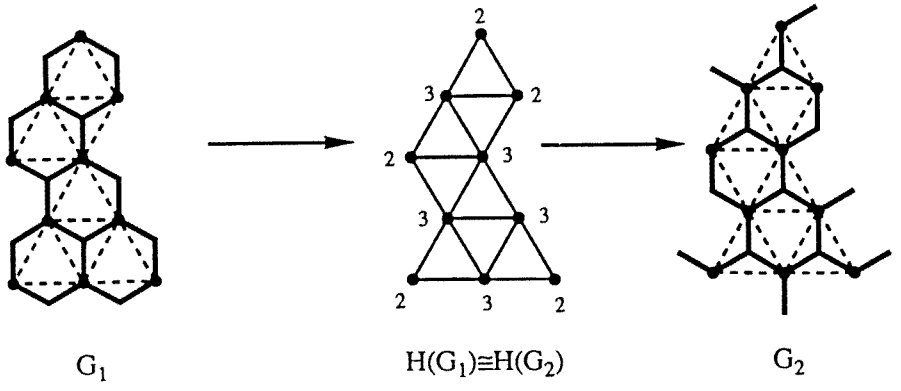


Fig. 1. An example of isospectral graphs constructed by Heilbronner's procedure. Vertices in G_1 and G_2 which are retained in their H-graphs are marked by heavy dots. Numbers at vertices of $H(G_1) \cong H(G_2)$ denote the respective number of loops. This example also presents an unsuccessful attempt to obtain a pair of IBGs by Heilbronner's original procedure.

One can hardly expect to obtain a pair of IBGs in this way by starting from a randomly chosen benzenoid graph G_1, since the reconstruction of $H(G_1)$ into

another benzenoid graph G_2 is rarely possible. For this reason, the recipe [5] does not follow the original scheme [7]. The conditions which $H(G)$ must fulfill in order to be reconstructable into two different benzenoid graphs are formulated [5] in terms of structural details of its dualist.

The dualist of the triangular graph $H(G)$, denoted as $D[H(G)]$, is defined analogously as for hexagonal graphs in [8,9]: $D[H(G)]$ is the geometrical object obtained from $H(G)$ by placing a point into the middle of each ring (in this case, a triangle) and by linking the points positioned in the rings sharing a common edge. Figure 2 illustrates the relationship between a benzenoid graph G and its derivatives $H(G)$ and $D[H(G)]$.

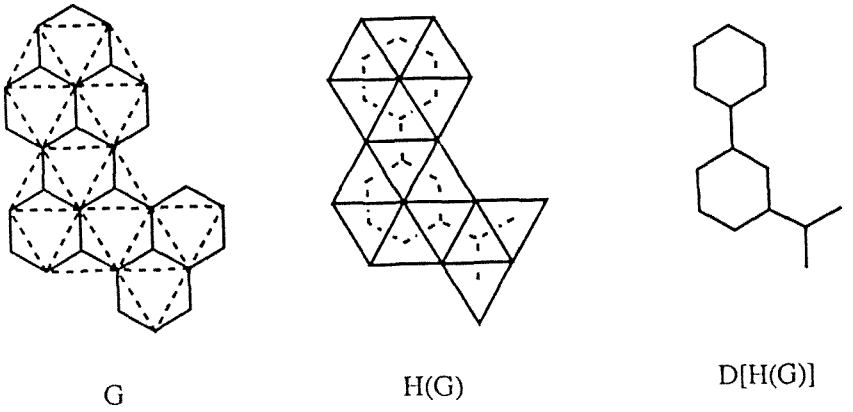


Fig. 2. A benzenoid graph G and its derivatives $H(G)$ and $D[H(G)]$. Dashed lines in G and $H(G)$ indicate the way of generating $H(G)$ and $D[H(G)]$, respectively.

When a dualist meeting the formulated requirements is chosen, the construction proceeds by deriving the appropriate $H'(G)$. This is done in a straightforward and unambiguous manner. Two IBGs are then reconstructed from $H'(G)$ in a few steps. Firstly, new vertices are added into nonadjacent triangles of $H'(G)$. Two complementary sets of triangles can be chosen for this purpose. Each inscribed vertex is linked to the three apices of the triangle, and the edges – sides of the triangle – are removed. After that, the old edges of $H'(G)$ remain only on the perimeter. Each of them is replaced by a new vertex linked to the vertices which were terminating the edge. The two graphs thus obtained are related by the two complementary sets of triangles into which new vertices were inscribed during the construction. An example in fig. 3 demonstrates the described procedure step-by-step.

The conditions which a dualist chosen for the construction of IBGs must satisfy have been given in [5]. A more complete list is given here:

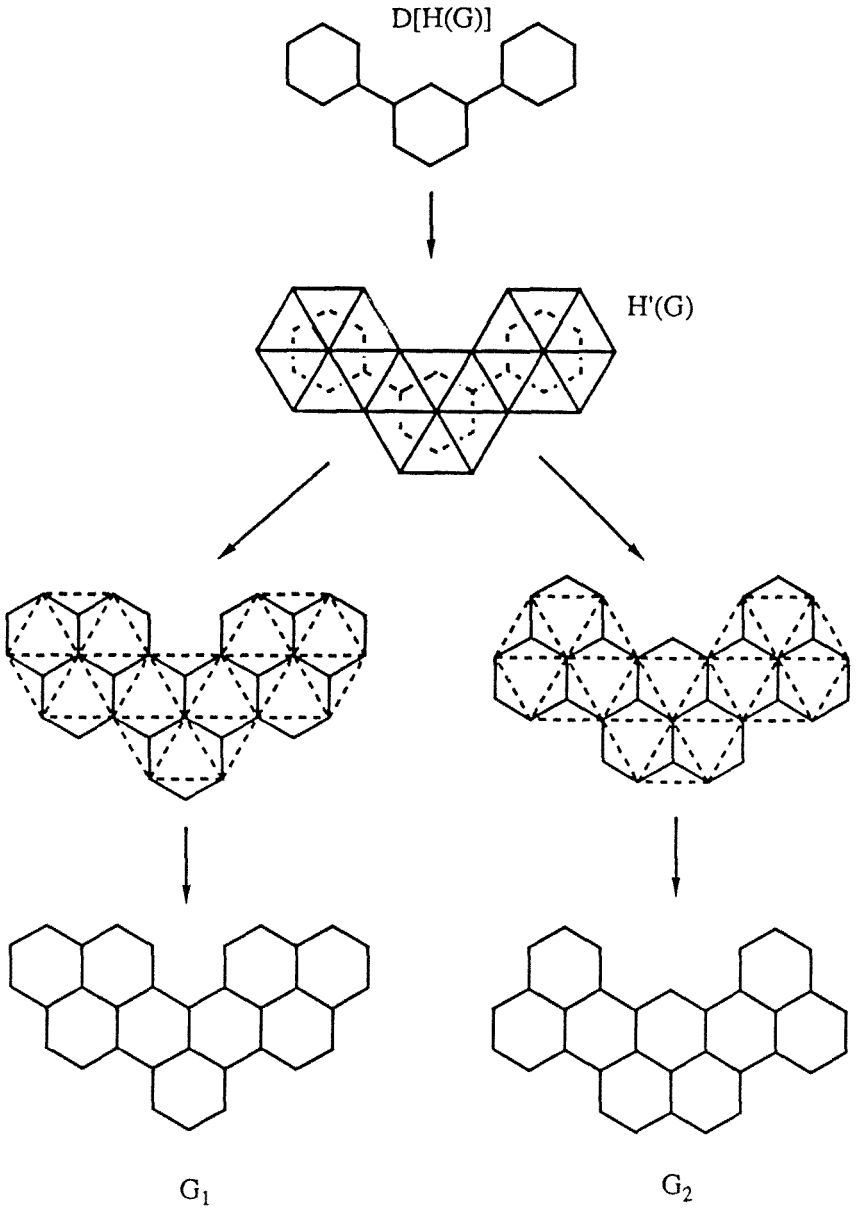


Fig. 3. An example of IBGs constructed by the Heilbronner-like procedure. G_1 and G_2 are the smallest existing pair of IBGs (with respect to the number of vertices and hexagons) as established by an exhaustive examination [10].

(i) The dualist must be embeddable into the hexagonal lattice.

(ii) If any two vertices of the dualist embedded in the hexagonal lattice are linked by a single edge or by a single vertex, this edge or vertex must also be contained in the dualist.

(iii) The dualist cannot contain any terminal vertex.

(iv) Hexagons are the only elementary cycles in the dualist.

(v) The structural details named M-fragments (see fig. 4) must be absent from the dualist.

(vi) The two vertex-colorings of the dualist (using two colors) must not be symmetry-equivalent.

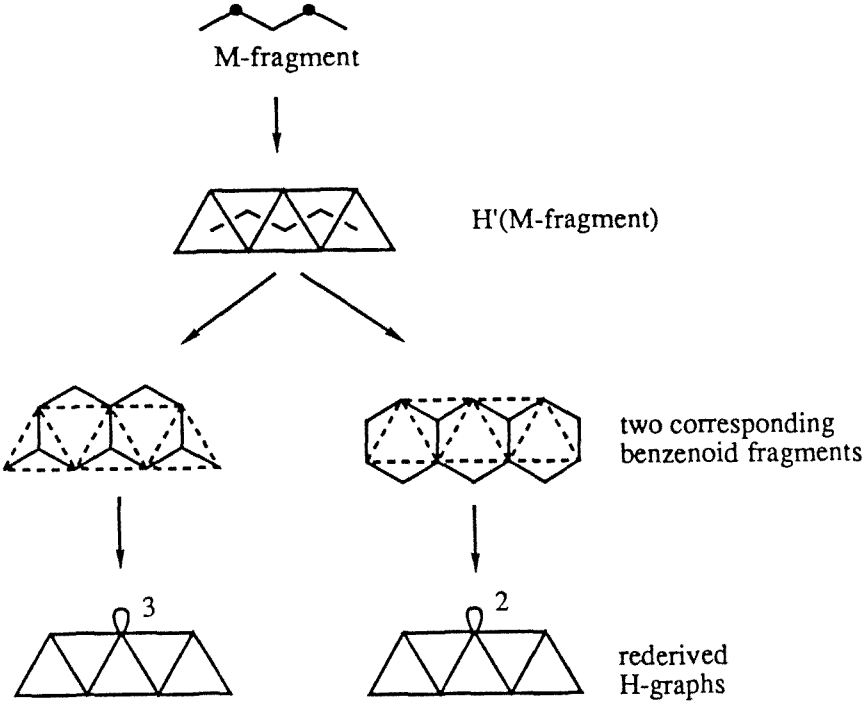
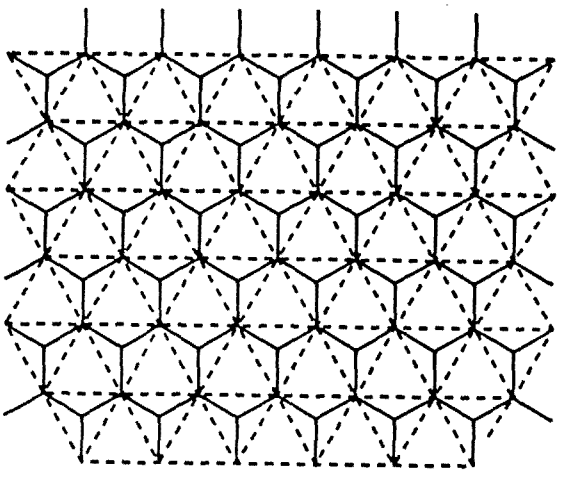


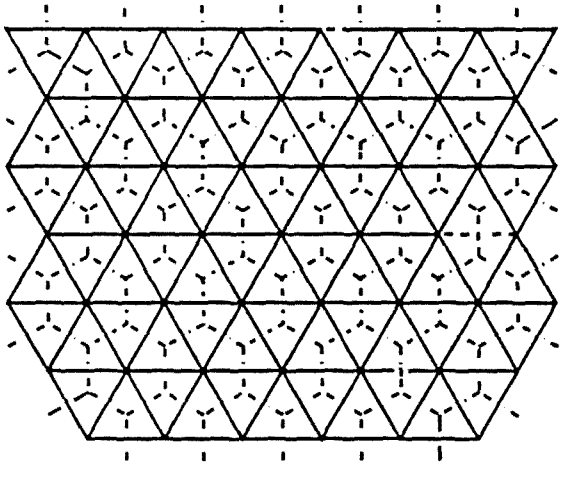
Fig. 4. The structural detail named M-fragment is forbidden in the dualist. The vertices marked by heavy dots are divalent, the others may be trivalent. The Heilbronner-like procedure transforms the M-fragment into two benzenoid fragments with different loop numbers on the corresponding vertices in their H-graphs.

3. The necessity of conditions (i)–(vi)

Recall that a benzenoid graph is a subgraph of the hexagonal lattice induced by the vertices lying on and inside the given cycle [9]. Figure 5(a) shows that an



(a)



(b)

Fig. 5. (a) An H'-graph of the hexagonal lattice (marked with a solid line) is the triangular lattice (marked with a dashed line). (b) The dualist of the triangular lattice (solid line) is the hexagonal lattice (dashed line).

H'-graph of the hexagonal lattice is the triangular lattice. $H'(G)$ is a subgraph of the triangular lattice in the same way as G is a subgraph of the hexagonal lattice: a cycle formed by connecting the next-nearest neighbors on the perimeter of G is embedded into the triangular lattice and the subgraph induced by the vertices lying on and inside the cycle is $H'(G)$. Figure 5(b) shows that a dualist of the triangular lattice is again the hexagonal lattice (now viewed as a geometrical object, not as a graph). Thus, $D[H(G)]$ of any benzenoid graph G is a part of the hexagonal lattice and therefore embeddable on this lattice.

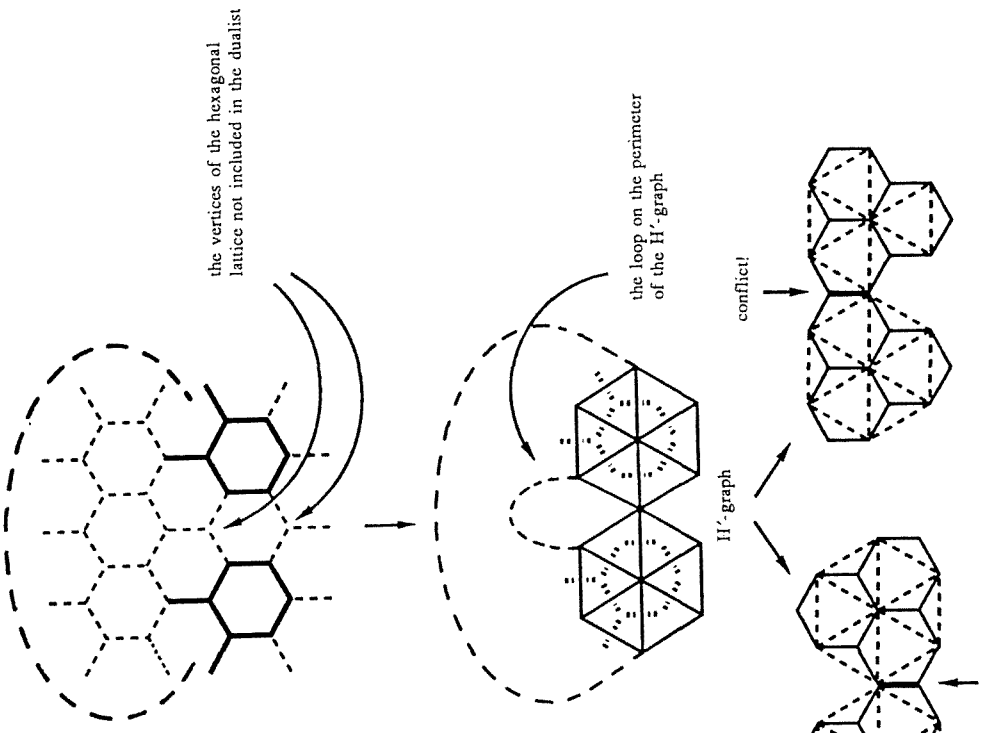


Fig. 6(b). Caption follows.

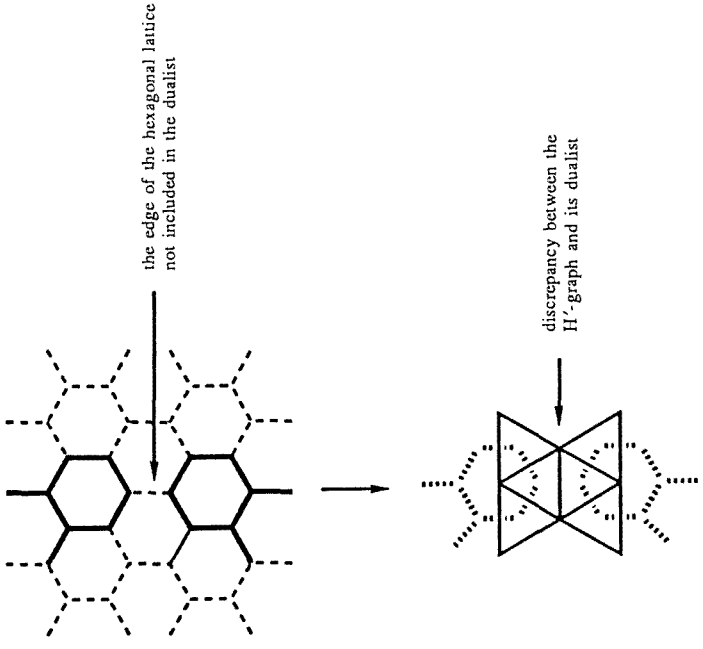


Fig. 6(a). Caption follows.

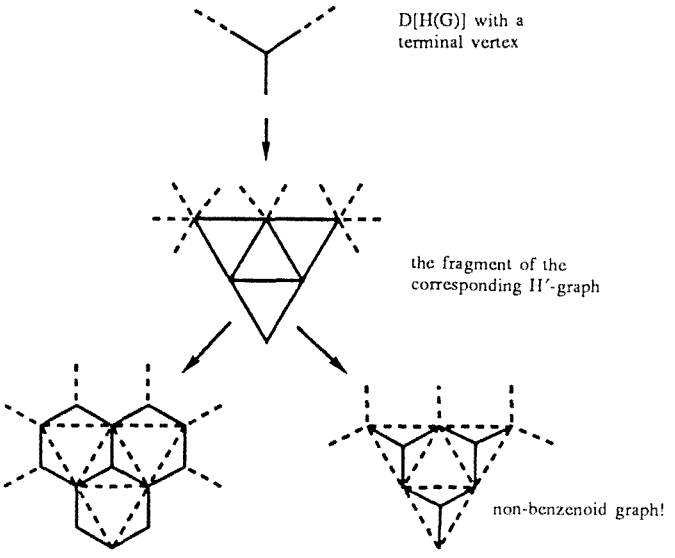


Fig. 6. The transformation of the three forbidden details in the dualist: (a) an edge of the hexagonal lattice between two vertices of the dualist; (b) a vertex of the hexagonal lattice between two vertices of the dualist; (c) a terminal vertex.

If an edge between two vertices is present in the hexagonal lattice but not in the embedded dualist, it is impossible to construct the appropriate H-graph, as is shown in fig. 6(a). If, instead of an edge, condition (ii) is violated in the same way by a vertex, it is not possible to transform the appropriate H-graph into two benzenoid graphs, as fig. 6(b) shows. A similar problem is present in the transformation of a terminal vertex of the dualist (fig. 6(c)).

According to the definition of a benzenoid graph [9], edges of the hexagonal lattice lying inside the perimeter of G are also in G. This holds not only for the perimeter, but for any cycle in G. This property applies also to $H(G)$ with respect to the underlying triangular lattice and to $D[H(G)]$ embedded on the hexagonal lattice. As a consequence, $D[H(G)]$ does not contain elementary cycles other than hexagons.

The last claimed condition requires that the dualist has two distinguishable vertex colorings with two colors. This means that the two different colorings of the dualist $D[H(G)]$ cannot be transformed into each other by means of some operation of the symmetry group of $D[H(G)]$. It was shown in [5] that a colored $D[H(G)]$ completely determines the way of its reconstruction into a benzenoid graph G (assuming that vertices of one of the two colors are chosen to represent the triangles of $H(G)$ into which vertices of G will be inscribed during the construction). Clearly, if the two colorings of $D[H(G)]$ are indistinguishable, so will the finally produced graphs: these will not only be isospectral, but isomorphic too.

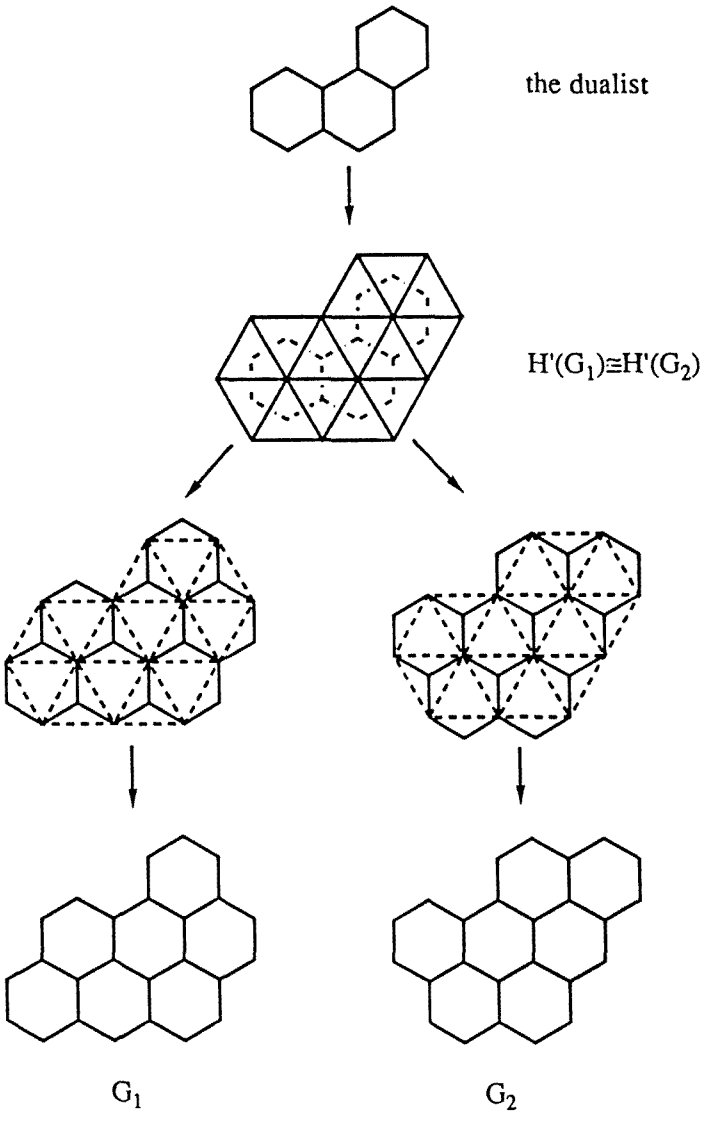


Fig. 7. The construction of IBGs starting from the dualist possessing M-fragments. The produced G_1 and G_2 are isomorphic.

Figure 4 depicts the way in which an M-fragment of the starting dualist is transformed into fragments of the final benzenoid graphs. Nothing opposes the regular way of the reconstruction, but a problem arises with different numbers of loops on the vertices of $H(G_1)$ and $H(G_2)$ designated in fig. 4. This difference brings into question the required isomorphism of $H(G_1)$ and $H(G_2)$. We prove that the isomorphism of $H(G_1)$ and $H(G_2)$ in this case implies the isomorphism of G_1 and

G_2, and thus represents the trivial solution. Assuming that the labeling of $H'(G)$ is retained in $H(G_1)$ and $H(G_2)$, the presumed isomorphism implies a permutation of labels by which $H(G_1)$ is mapped into $H(G_2)$. This isomorphism is not the trivial one, because the vertices related to an M-fragment have different numbers of loops in $H(G_1)$ and $H(G_2)$. This represents an automorphism of $H'(G)$ which involves a cyclic permutation of vertices related to M-fragments of $D[H(G)]$. By this permutation, the vertex of $H'(G)$ having three loops in, for example, $H(G_1)$ is mapped into the vertex with two loops in $H(G_2)$, and vice versa. It follows that the triangles in $H'(G)$ being "full" during the construction are mapped into those which are "empty". Bearing in mind the correspondence between the "full" and the "empty" triangles in $H(G)$ and vertex colors in $D[H(G)]$, the automorphism of $H'(G)$ implies the automorphism of $D[H(G)]$ by which all vertices of one color are mapped into those of another. Thence, the two colored $D[H(G)]$ cannot be distinguished and G_1 and G_2 obtained from them must be isomorphic. Figure 7 provides an illustrative example.

The necessity of conditions (i)–(vi) is thereby proven. Before examining their sufficiency, we assert some propositions which will be useful in the further consideration. They also enable an important conclusion about the limitation of the Heilbronner-like procedure when it is applied to the construction of IBGs.

4. IBGs with an even number of vertices cannot be constructed by the Heilbronner-like procedure

The perimeter of a benzenoid graph can be considered as a series of di- and trivalent vertices. A benzenoid graph is completely determined by specifying this sequence [11]. The subsequences of only trivalent vertices characterize the structural details of the perimeter known as fissure, bay, cove and fjord [9], with one, two, three and four consecutive trivalent vertices, respectively. Let us prove the following theorem about the minimal number of odd-length sequences.

THEOREM 1

A benzenoid graph cannot have only one odd-length sequence of trivalent vertices on its perimeter.

Proof

Let us write down the perimeter as a series $d_1t_1d_2t_2 \ldots d_pt_p$, where d_i and t_i denote the number of consecutive di- and trivalent vertices, respectively. This sequence should be started by counting at any divalent vertex preceded by the trivalent vertex. Let us define

$$\Delta_2 = n_2(\text{black}) - n_2(\text{white}),$$

$$\Delta_3 = n_3(\text{black}) - n_3(\text{white}),$$

$$\Delta = n(\text{black}) - n(\text{white}) = \Delta_2 + \Delta_3,$$

with n_d(color) denoting the number of d-valent vertices having the specified color in G.

First we derive a relation between Δ, Δ_2 and Δ_3. Each edge in a colored benzenoid graph joins a black vertex with a white vertex. Therefore, the number of edges incident to black vertices equals the number of edges incident to white vertices:

$$3n_3(\text{black}) + 2n_2(\text{black}) = 3n_3(\text{white}) + 2n_2(\text{white}).$$

A regrouping of terms in the last equation gives:

$$3\Delta_3 = -2\Delta_2 \Rightarrow \Delta_3 = -2/3\Delta_2.$$

By recalling the definition of Δ and by substitution of the Δ_3 term, one obtains:

$$\Delta = \Delta_2 + \Delta_3 = \Delta_2 - (2/3)\Delta_2 = \Delta_2/3.$$

This result implies that: (i) Δ can be determined by considering only the perimeter of a benzenoid graph, and (ii) Δ_2 must be a multiple of 3, i.e. the possible values of Δ_2 are $0, \pm 3, \pm 6, \ldots$.

Let us determine Δ_2 by considering the aforementioned series $d_1t_1d_2t_2 \ldots d_pt_p$. In order to derive Δ_2, the series is compressed in the following way. First, all even fragments d_i and t_i are omitted from the series. These fragments contain equal numbers of black and white vertices and do not affect the starting color in the next fragments, hence their presence can be ignored. Second, in the resulting sequence, all d-fragments, now consecutive, and t-fragments, now consecutive, are replaced by their sums. The result is a series of the same form as the starting one, but shorter. The compression is repeated until the sequence remains unchanged. It has the form $d_1't_1'd_2't_2' \ldots d_q't_q'$, where all d_i' and t_i' are exclusively odd numbers. One should note that, when colored, all d'-fragments in the series have an excess of the same color in the amount of exactly 1 vertex. Therefore, $|\Delta_2| = q$.

If the perimeter were imagined to have only one t-sequence of an odd length, the compression would yield $q = 1$, and consequently $\Delta_2 = \pm 1$. However, as our previous consideration shows, this is an impossible value for Δ_2. □

PROPOSITION 2

A dualist which satisfies conditions (i)–(vi) has an even number of vertices.

Proof

First we prove that each vertex in the valid dualist (one satisfying the stated conditions) belongs to at least one hexagon. According to condition (iv), a vertex which would not be in a hexagon could not be in any other cycle either. Thus, the vertices of the dualist could be partitioned into cyclic and acyclic vertices. A graph-induction by only cyclic vertices generates a (disconnected) "subdualist" whose

components are, in a graphical sense, linked benzenoids [12]. A linked benzenoid is produced by linking two (possibly also linked) benzenoids by a single edge, provided that the resulting graph is embeddable into the hexagonal lattice. The dualist in fig. 3 is an example of a linked benzenoid dualist.

The notion of the perimeter, common to benzenoid graphs, can be extended to a linked benzenoid dualist by considering the present bridges as two-membered cycles. The perimeter is traced while keeping the side on which an "inside" of the dualist is positioned. The structural details on the perimeter; fissure, cove and fjord, are defined in the usual way [9,12].

When applied to a pure benzenoid dualist, conditions (ii) and (v) are equivalent to forbidding the presence of fissures, coves and fjords on the perimeter. A fissure corresponds to an M-fragment, while fjord and cove imply the edge and the vertex, respectively, not allowed by condition (ii). The way in which a bridge links two (linked) benzenoid parts B_1 and B_2 in the valid dualist is depicted in fig. 8. One should note that the presence of a link between B_1 and B_2 does not affect the fulfillment of criterion (v) when applied to separate B_1 or B_2.

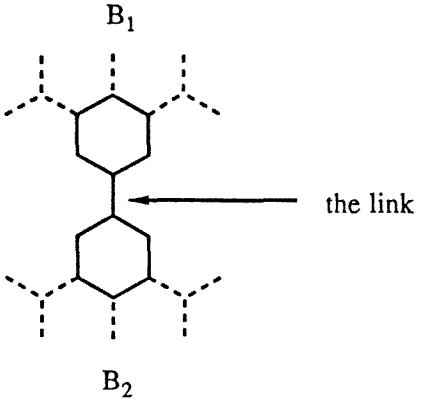


Fig. 8. The fragment of the valid dualist containing a bridge between two hexagons.

A dualist possessing an acyclic vertex can be transformed into a tree by substituting each linked benzenoid component by a single vertex. Due to condition (iv), each terminal vertex in the resulting tree must correspond to some linked benzenoid component of the starting dualist, connected to a single acyclic vertex. An inspection shows that because of conditions (ii) and (v), the acyclic vertex must be divalent and linked to a cyclic component in a way depicted in fig. 9. The shown fragment indicates that a separate benzenoid component needs to possess a fissure near the vertex which is to be linked with an acyclic vertex. This fissure should be the only odd-length sequence of trivalent vertices on the perimeter of the corresponding

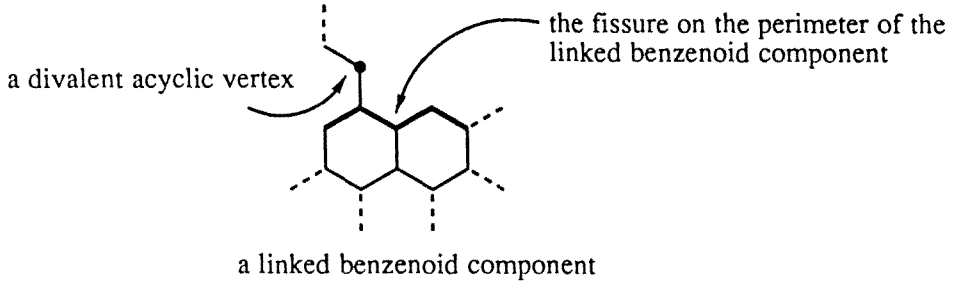


Fig. 9. The fragment of the (hypothetical) valid dualist with a cyclic component linked to a single acyclic vertex.

benzenoid part of the dualist. However, from theorem 1 we know that such a benzenoid does not exist, and therefore a linked benzenoid component cannot be connected to a single acyclic vertex. This further implies that the valid dualist cannot possess an acyclic vertex and that it must be, in a graphical sense, a linked benzenoid.

It has been shown in [12] that a necessary and sufficient condition for a (linked) benzenoid to be an all-benzenoid graph [9] is the absence of fissures and coves on the perimeter. Since conditions (ii) and (v) forbid the presence of fissures and coves (and fjords) on the perimeter, the linked benzenoid corresponding to the valid dualist must be an all-benzenoid graph. Therefore, the number of vertices in the valid dualist is a multiple of 6 and, of course, an even number. □

Now conditions (i)–(v) can be expressed in a more concise manner. The dualist being, in a graphical sense, a linked benzenoid graph without fissures, coves and fjords, automatically satisfies conditions (i)–(v), and only condition (vi) needs to be accounted for separately.

PROPOSITION 3

Let G be a benzenoid graph with h hexagons and let Δ denote its color excess [9]. Then the number of vertices N in $D[H(G)]$ equals

$$N = 2h - 1 + \Delta \quad \text{or} \quad N = 2h - 1 - \Delta.$$

Proof

N is equal to the number of triangles in $H(G)$. When $H(G)$ is constructed from the colored G, one finds that a triangle is created in each hexagon and around non-adjacent trivalent vertices in G. Two graphs $H(G)$ are possible and the respective numbers of triangles in them N_1 and N_2 are:

$$N_1 = h + n_3(\text{white}), \quad N_2 = h + n_3(\text{black}),$$

where h denotes the number of hexagons in G. The following relation is known [9]:

$$n_3(\text{black}) + n_3(\text{white}) = 2h - 2$$

and from the proof of theorem 1, one obtains

$$n_3(\text{black}) - n_3(\text{white}) = \Delta_3 = -2\Delta.$$

From the last two equations, one easily arrives at:

$$n_3(\text{white}) = h - 1 + \Delta, \quad n_3(\text{black}) = h - 1 + \Delta.$$

Substitution into the expressions for N_1 and N_2 gives the formulas stated in the proposition. □

An important consequence of the two propositions is:

COROLLARY 4

An isospectral pair of benzenoid graphs G_1 and G_2, each with an even number of vertices, if existent, does not possess an isomorphic pair $\{H(G_1), H(G_2)\}$, i.e. it cannot be obtained by the Heilbronner-like procedure.

Proof

We have proven that conditions (i)–(v) are necessary in order for G_1 and G_2 to have an isomorphic pair $\{H(G_1), H(G_2)\}$. By proposition 2, the number N of vertices in $D[H(G)]$ is even. Then from proposition 3, it follows that Δ must be an odd number, and this is possible only if G has an odd number of vertices. □

PROPOSITION 5

Benzenoid graphs G_1 and G_2 having an isomorphic pair $\{H(G_1), H(G_2)\}$ must have an equal number of vertices.

Proof

Let n denote the number of vertices in a benzenoid graph G and let n_i be the number of internal vertices in G. Let p be the size of the perimeter and h be the number of hexagons in G. The number of edges in G is denoted by m. The following formulas may be found in [9]:

$$n = 4h + 2 - n_i,$$
$$m = n + h + 1,$$
$$p = 4h + 2 - 2n_i.$$

From them, one obtains

$$n = (4m + p + 6)/6.$$

G_1 and G_2 must have an equal number of edges (m), since m is determined by the sum of the numbers of loops on the vertices of $H(G_1) \cong H(G_2)$. From the relation between G and $H(G)$, it is clear that the perimeter of G is twice as large as the perimeter of $H(G)$. Thence, the perimeters of G_1 and G_2 are of equal size (p). By the latter equation, they must also have an equal number of vertices (n). □

5. The necessary conditions for the construction of IBGs by the Heilbronner-like procedure are also sufficient

In order to prove that conditions (i)–(vi) are not only necessary but also sufficient, we have to verify that their fulfillment guarantees that two non-isomorphic IBGs will be obtained by the described procedure. The three required properties of the constructed graphs: benzenoid character, isospectrality and non-isomorphism, are examined separately.

From the relationship between the triangular lattice and its dualist – the hexagonal lattice, shown in fig. 5(b) – it is clear that the dualist can be placed on the triangular lattice so that every one of its vertices occupies a triangle. The H'-graph is obtained as a subgraph of the triangular lattice induced by the vertices of the occupied triangles. Pathological situations can arise in only two ways: if the perimeter of the H'-graph contains the closed loop, and if two vertices nonadjacent in the dualist correspond to two adjacent triangles in the H'-graph. Since terminal vertices are not allowed in the dualist, the first situation occurs only in the way depicted in fig. 6(b). An inspection of the underlying fragments in the dualist reveals that both situations are prevented by condition (ii). Hence, the construction of the H'-graph with a well-defined parameter is assured.

An H'-graph can be placed on the hexagonal lattice in two different ways so that the vertices overlap. The two possible placements are related by a shift of the H'-graph along a single edge in the hexagonal lattice. In order to derive a benzenoid graph from the H'-graph, it is sufficient to reconstruct its perimeter. The inner part can be obtained by the induction of edges lying between vertices on and inside the perimeter. Figure 10 depicts the reconstruction around vertices of various degrees in an H'-graph. In all allowed situations, the reconstruction of the perimeter proceeds smoothly in both projected ways. Thus, the two graphs produced by the described procedure will be of benzenoid character provided the starting dualist obeys conditions (i)–(iv).

Figure 10 also shows that the vertices of the H'-graph, when they become a part of the derived benzenoid graphs, have equal numbers of neighbors in both constructed graphs G_1 and G_2. Therefore, the numbers of loops on the vertices of an H'-graph derived from either of the two constructed graphs are the same. This

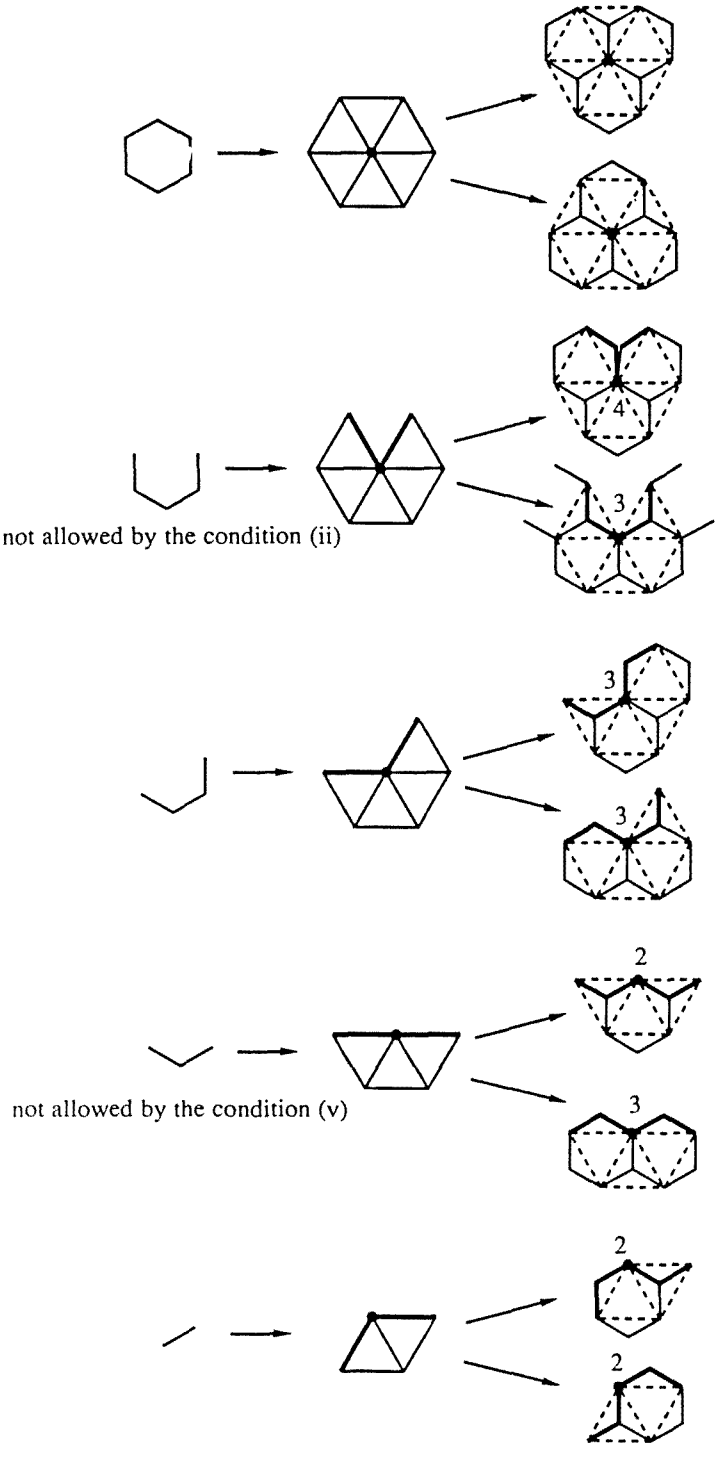


Fig. 10. The vertices of various degrees in an H'-graph are depicted in the middle column. In the left-most column are shown the parent fragments of the dualist, while the right-most column shows the constructed fragments of a benzenoid graph. The top-most row represents an inner vertex; all others are on the perimeter. Heavy lines indicate the perimeter edges. Numbers at the heavy-dot vertices are equal to the number of loops in the respective H-graph.

means that the two H'-graphs $H(G_1)$ and $H(G_2)$ are isomorphic. By proposition 5, G_1 and G_2 have an equal number of vertices, and by theorem in [7], they must be isospectral.

It remains to be shown that the fulfillment of the prescribed conditions guarantees that the two constructed graphs will not be isomorphic. We do this by proving that the isomorphism in this case implies the violation of condition (vi). Let us color the vertices in G_1 and G_2 so that those which originate from the common H'-graph have equal colors in both G_1 and G_2. The presumed isomorphism maps the vertices of G_1 onto those of G_2 so that the color of all vertices is either kept the same or changed into the opposite one. The last possibility must be abandoned since it implies the same number of the two kinds of colored vertices, which cannot be true by corollary 6. Therefore, the vertices from G_1 originating from the H'-graph are mapped onto the same ones in G_2. The triangles which were chosen as "empty" for generating G_1 must be mapped onto the "empty" triangles in G_2. This means that the considered isomorphism represents an automorphism of the H'-graph which interchanges the two complementary sets of triangles. Bearing in mind their correspondence with the colored vertices in $D[H(G)]$, it follows that the two vertex colorings of $D[H(G)]$ are equal.

6. Conclusions

The procedure presented in [5] exhausts the possibilities for the construction of IBGs on the basis of isomorphic H-graphs, i.e. by the Heilbronner-like procedure.

There is no pair of isospectral benzenoid graphs each with an even number of vertices having a pair of isomorphic H-graphs.

It has been ascertained in section 4 that the valid dualist corresponds to a linked benzenoid graph which can be partitioned into disjoint hexagons [12]. This is in parallel with the observation reported in [5] that the isospectral benzenoid pairs generated by the Heilbronner-like procedure can be viewed as being built from phenalene tiles. Characteristics of the phenalene graph relevant for the construction of isospectral pairs have already been studied in [13]. Each phenalene tile corresponds to a separate hexagon in the dualist $D[H(G)]$, and the "upside-down" procedure [5] can be viewed on the dualist level as a transition from one to another colored dualist. This leads to the conclusion that the Heilbronner-like procedure for the construction of isospectral benzenoid graphs is equivalent to building them from phenalene tiles by using the "upside-down" transformation. However, this interpretation will be considered in a separate paper.

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References

[1] M. Randić, M. Barysz, J. Nowakowski, S. Nikolić and N. Trinajstić, J. Mol. Struct. (THEOCHEM) 185(1989)95.
[2] Y. Jiang and C. Liang, On endospectral bipartite graphs, *9th Int. Conf. on Mathematical and Computational Chemistry*, Bled, Yugoslavia (1991).
[3] O. Ivanciuc and A.T. Balaban, Nonisomorphic graphs with identical atomic counts of self-returning walks, ibid.
[4] Ch. Rücker and G. Rücker, J. Math. Chem., in press.
[5] D. Babić, J. Math. Chem, in press.
[6] J. Cioslowski, J. Math. Chem. 6(1991)111.
[7] E. Heilbronner, MATCH 5(1979)105.
[8] F.T. Smith, J. Chem. Phys. 34(1979)105;
A.T. Balaban and F. Harary, Tetrahedron 24(1968)2505.
[9] I. Gutman and S.J. Cyvin, *Introduction to the Theory of Benzenoid Hydrocarbons* (Springer, Berlin, 1989).
[10] I. Gutman, S. Marković and V. Grbović, J. Serb. Chem. Soc. 56(1991)553;
S.J. Cyvin, private communication.
[11] W.C. Herndon and A.J. Bruce, in: *Graph Theory and Topology in Chemistry*, ed. R.B. King and D.H. Rouvray (Elsevier, New York, 1987), pp. 491–513.
[12] I. Gutman and D. Babić, J. Mol. Struct. (THEOCHEM) 251(1991)367.
[13] W.C. Herndon and M.L. Ellzey, Jr., Tetrahedron 31(1975)99.