Isospectral benzenoid graphs with an odd number of vertices

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A procedure for construction of isospectral pairs of benzenoid graphs is described. It is based on the Heilbronner "wrapping" procedure for construction of isospectral bipartite graphs. Only isospectral pairs having an odd number of vertices could be produced (the smallest among them has 33 vertices and 9 hexagons). Thus, the conjecture announced by Cioslowski is partially disproved.

1. Introduction

The work reported here has been motivated by the recently announced conjecture [1] on non-existence of isospectral benzenoid graphs. In the present paper, this conjecture is partially disproved by counterexamples having an odd number of vertices. Here is described a procedure by which further isospectral benzenoid pairs can be constructed. However, it is confined exclusively to benzenoids with an odd number of vertices. Thus, the conjecture stated in ref. [1] still holds when restricted to benzenoids with an even number of vertices.

For graph-theoretical definitions and nomenclature, the reader is referred to refs. [2,3]; only necessities will be given here. A benzenoid graph is defined [3] as a graph induced by the vertices lying on and inside the cycle in the hexagonal lattice. A spectrum of the graph G denotes a set of eigenvalues of the corresponding adjacency matrix $A(G)$. Non-isomorphic graphs having equal spectra are called isospectral. In the following text, the terms "benzenoid graph" and "isospectral benzenoid graphs" will be shortly written as BG and IBGs, respectively.

The present procedure for construction of IBGs essentially relies on the method reported by Heilbronner [4]. It is, in fact, the Heilbronner method adapted just for benzenoid graphs: some additional rules ensure that the obtained graphs will be benzenoid and non-isomorphic.

2. Heilbronner's procedure

By Heilbronner's procedure, only bipartite isospectral graphs can be constructed. The vertices of a bipartite graph can be colored with two colors so that no two neighbors are equally colored. If vertices of one color are numbered first, and then the remaining vertices of another color, the corresponding adjacency matrix and its square will have the following forms:

$$A(G)=\begin{bmatrix} 0 & B \\ B^{\mathrm{T}} & 0 \end{bmatrix}, \quad A^2(G)=\begin{bmatrix} BB^{\mathrm{T}} & 0 \\ 0 & B^{\mathrm{T}}B \end{bmatrix}.$$

Diagonal blocks of $A^2(G)$ can be regarded as adjacency matrices of two smaller graphs derived from the parent graph G. They can also be constructed directly from G by first removing all vertices of one chosen color (together with all edges), and then by linking the retained vertices. Each two retained vertices are to be linked by as many edges as they had common neighbors in G. In addition, each vertex gets as many loops as it had neighbors in G. Any of the two graphs obtained in this way will be called an H-graph of G and denoted as $H(G)$. An H-graph with loops removed will be denoted as $H'(G)$ and called a truncated H-graph.

If two non-isomorphic bipartite graphs G_1 and G_2 with an equal number of vertices have at least one isomorphic pair $\{H(G_1), H(G_2)\}$, then G_1 and G_2 are isospectral [4]. Heilbronner's procedure relies on the fact that a reconstruction of G from a given $H(G)$ is not in general unique. It begins with the construction of an H-graph from a given G_1. Then from $H(G_1)$ one attempts to reconstruct a different parent graph G_2. If it is possible, and if G_1 and G_2 have an equal number of vertices, they are isospectral. An illustrative example is given in fig. 1.

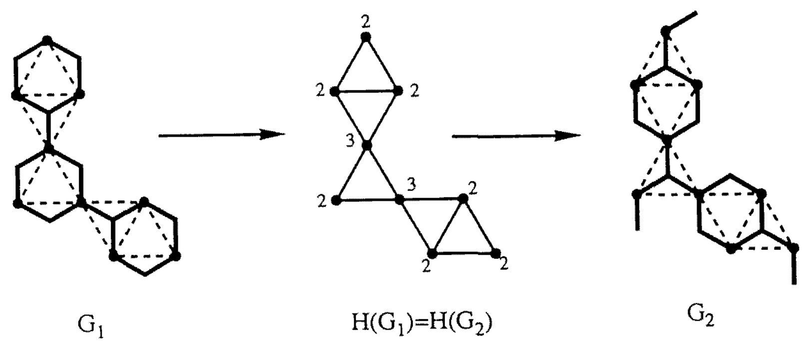

Fig. 1. An example of isospectral graphs constructed by the Heilbronner procedure. The vertices in G_1 and G_2 retained in their H-graph are marked by boldface. Numbers at vertices of $H(G_1) = H(G_2)$ denote the associated number of loops.

3. Specialization for benzenoid graphs

Let us consider a relation between a benzenoid and its H-graph. As fig. 2 shows, a truncated H-graph of the hexagonal lattice (HL) is the triangular lattice (TL). A truncated H-graph of the benzenoid graph G is a subgraph of the TL in the

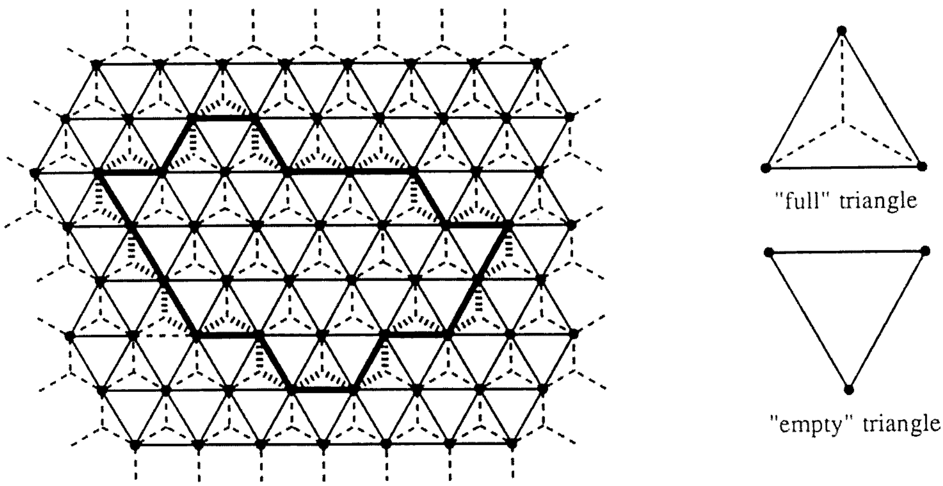

Fig. 2. A truncated H-graph of the hexagonal lattice is the triangular lattice. A perimeter of an example BG and of the corresponding H'(BG) are drawn by bold dotted and full lines, respectively. Details termed as "full" and "empty" triangles are drawn, enlarged, on the right-hand side.

same way as G is a subgraph of the HL: $H'(G)$ is a graph induced by vertices of the TL lying on and inside the perimeter of the underlying G.

During a reconstruction, $H'(G)$ is being "wrapped" by adding new vertices [4]. Figure 2 reveals an important feature of reconstruction of a benzenoid graph G from a given $H'(G)$: new vertices are added by inscription into the triangles of $H'(G)$ in a strictly alternative manner: each "full" triangle (with a new vertex inscribed) shares its edges only with "empty" triangles (without a new vertex), and vice versa: each "empty" triangle is surrounded only by "full" triangles. This shows that from a given $H'(G)$, one can try to reconstruct the parent benzenoid graph(s) in two and only two ways related to the two mutually exclusive sets of triangles into which new vertices will be inscribed.

The reconstruction process is completely determined once the first new vertex is inscribed into $H'(G)$. It fixes positions at which all other vertices will be added. After new vertices are inscribed, each of them is linked to the vertices of the proper triangle, and old edges – sides of the triangle – are erased. After that, original edges of the $H'(G)$ are present only on its perimeter. Each one is to be replaced by a new vertex linked to the vertices which were ending the replaced edge.

In the original Heilbronner procedure, one starts with a given graph G_1 and, by using $H(G_1)$, eventually derives an isospectral mate G_2. However, since IBGs are rather rare, one can hardly expect to find such a pair accidentally. Instead, one is prompted to look for such $H(G)$ from which both of the two ways of reconstruction will be possible. This task is fairly complicated by loops present in $H(G)$, and for this reason the search is further shifted onto an appropriate $H'(G)$.

A truncated H-graph, which we are looking for, must satisfy the following conditions: it must allow a reconstruction of a parent graph in both of the two ways, the two obtained graphs must be benzenoid, non-isomorphic and with an equal number of vertices, and their complete H-graph must be isomorphic. An examination of a few examples quickly leads to the formulation of some necessary conditions. These conditions require the absence of certain structural details in $H'(G)$ and are best explained in terms of its dualist $D(H')$.

A dualist of a triangular graph is defined in the same way as for a BG [5]: a graph is first embedded in the TL, and in the center of each triangle a vertex of the dualist is placed. The vertices in adjacent triangles are linked, and upon completion, the dualist is obtained. Angles between edges are held fixed, and thus a dualist is

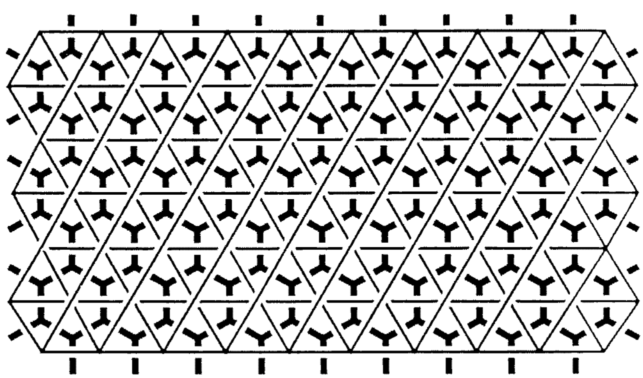

Fig. 3. A triangular lattice (normal line) and a hexagonal lattice (bold line) positioned as dualist graphs of each other.

not a graph, but rather a geometrical object. As fig. 3 shows, a dualist of the TL is again the HL (and vice versa). Therefore, a dualist of $H'(G)$ must be embeddable into the HL.

Figure 4 shows three structural details which are forbidden in the dualist $D(H')$. Figure 4(a) shows that $D(H')$ cannot have any terminal vertex since the corresponding triangular graph cannot be reconstructed into a valid BG when a triangle which corresponds to a terminal vertex of $D(H')$ is chosen to be "full". The same applies to a detail depicted in fig. 4(b): one of the two reconstuction ways cannot yield a valid BG.

A detail shown in fig. 4(c) is related to the loops of an H-graph. Let us recall that an isospectrality of the constructed BGs is guaranteed when their complete, not only truncated, H-graphs are isomorphic. When the detail from fig. 4(c) is present in a dualist, the two H-graphs will have a different number of loops on the designated vertex. Although this does not mean that the two complete H-graphs will be non-isomorphic, the eventual isomorphism in this case did not prove to be useful: in all considered examples, the two constructed BGs were found to be isomorphic too.

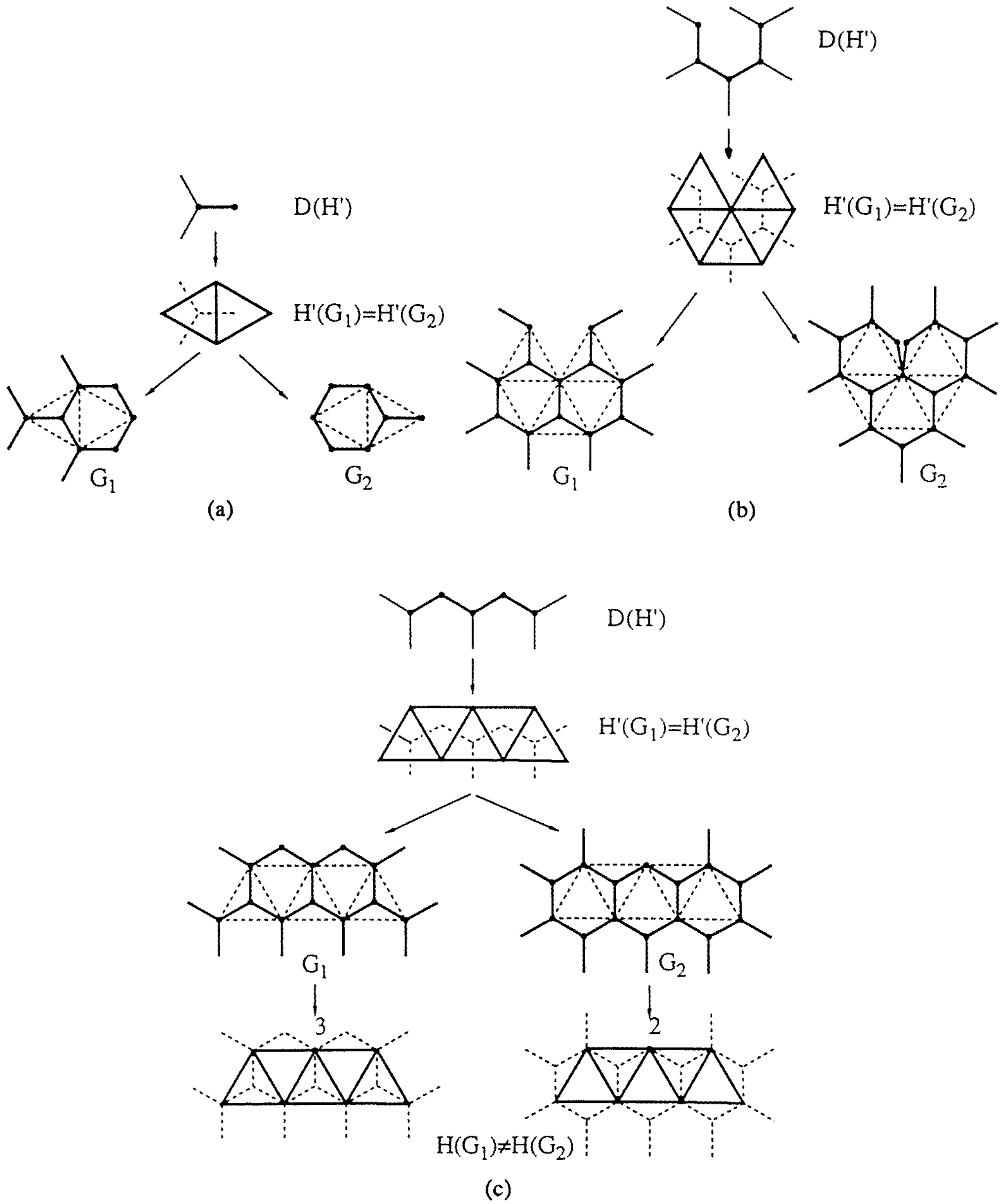

Fig. 4. (a) $D(H')$ must not possess a terminal vertex. In the case of its presence, at most one way of reconstruction is possible: G_2 possesses a terminal vertex and therefore is not a BG. (b) The detail of $D(H')$ which can be reconstructed also in at most one way: G_2 contains the four-valent vertex improper to a BG. (c) The detail of $D(H')$ and its two ways of reconstruction into G_1 and G_2. It is forbidden because $H(G_1)$ and $H(G_2)$ have different numbers of loops at the designated vertex.

In order to avoid an isomorphism of the graphs being constructed, an additional condition is put on the dualist $D(H')$. According to its relation to the HL, vertices of $D(H')$ can be colored with two colors so that no two adjacent vertices would be of the same color. Two such colorings of $D(H')$ are possible. If the two colored dualists are equal, the constructed benzenoid graphs will be isomorphic. This is clear from the following consideration. Vertices of one color may be taken to represent triangles which will be full during the construction. Then the colored $D(H')$ determines the parent H'-graph, and also the way of its use in the construction. If the two colored $D(H')$ are indistinguishable, so will be also the BGs derived from them.

Hence, the conditions formulated so far require that the dualist $D(H')$: (1) must be embeddable into the HL, (2) has no terminal vertices, (3) has no details shown in figs. 4(b) and (c), and (4) has two different vertex colorings in two colors. The present conditions are shown to be necessary. Whether they are also sufficient remains to be proven [6].

4. Examples

Since the required conditions are formulated in terms of a dualist $D(H')$, a natural way to begin a construction is to find a satisfactory dualist. Each BG without fissures, coves and fjords on its perimeter (see ref. [3] for definitions of these structural details) is a good candidate for a valid dualist. It has only to be checked on different colorings. All other conditions are already fulfilled.

A useful extension of this class has been found in the so-called, linked benzenoids. These are graphs obtained by linking separate (possibly also linked) benzenoid systems by bridges, so that the resulting graph is again embeddable in the HL. If the notion of perimeter is extended to comprise the present bridges too, linked benzenoids can also be characterized by structural details such as fissures, bays, coves and fjords. In order to be a valid $D(H')$, also the linked benzenoid graph must not possess fissures, coves and fjords, and must have two different colorings. No other kind of graphs could be found to satisfy the established criteria. Figure 5 shows some examples of valid dualists $D(H')$.

Figure 6 depicts an example of the construction of IBGs. Incidentally, the two benzenoid graphs shown are the isospectral pair with the least number of hexagons (nine) obtained to date. Whether it is the smallest one will be clear after a systematic examination is completed [7].

5. Closing remarks

The described procedure can be used for systematic generation of IBGs. Although a necessity and sufficiency of the specified rules are not strictly proven, they can at least serve as a good guideline.

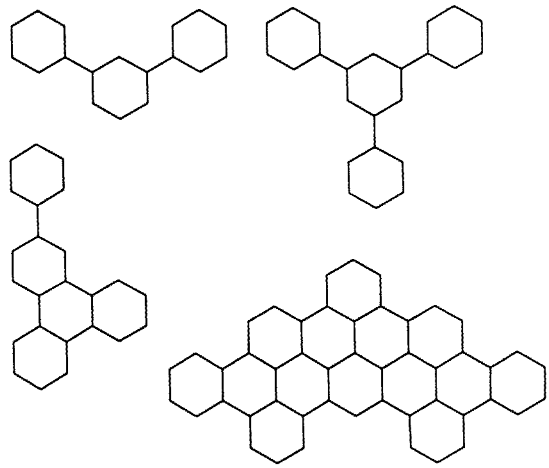

Fig. 5. Examples of valid $D(H')$ graphs: they are distinctly (linked) BGs without fissures, coves and fjords on their perimeters and with two different colorings in two colors.

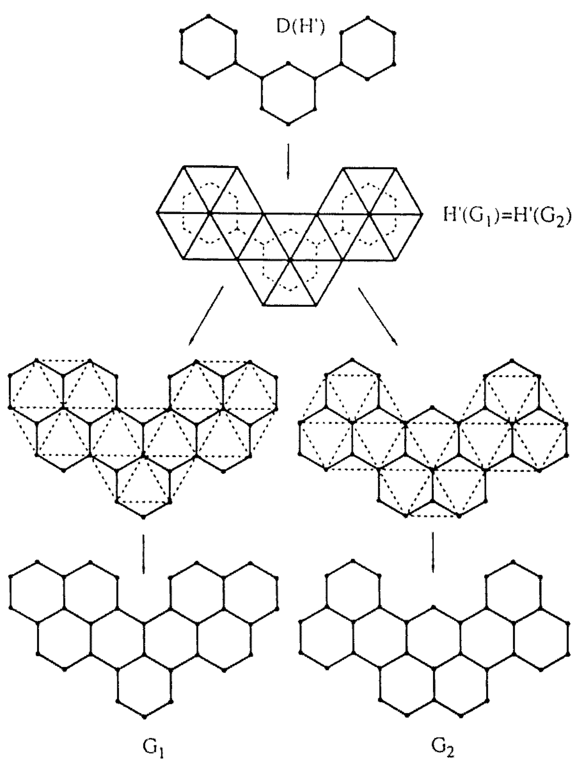

Fig. 6. An illustration of the described procedure for construction of IBGs. The shown example is with the least number of hexagons obtained to date.

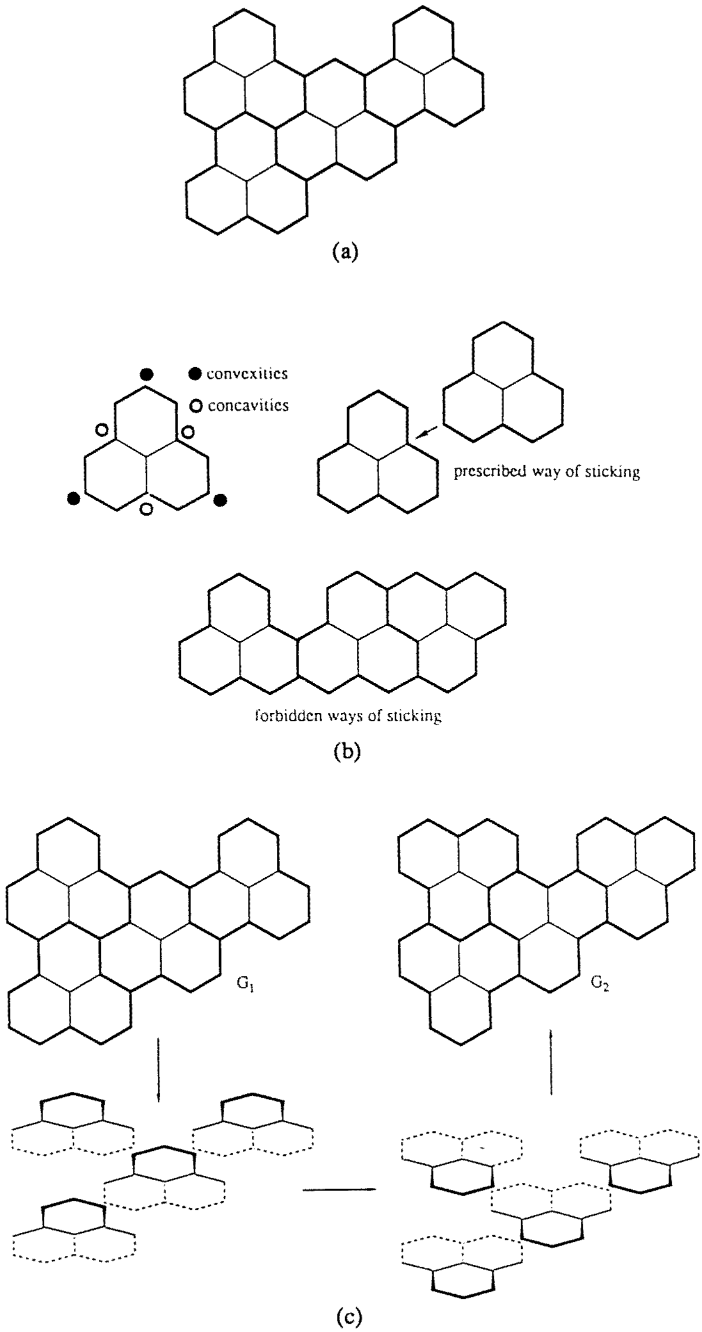

Fig. 7. (a) BG composed from phenalene tiles. (b) On the first drawing, convexities (full circles) and concavities (empty circles) of a phenalene tile are designated. The second drawing depicts the prescribed way of sticking of adjacent tiles, and the third drawing depicts disallowed ways of their sticking. (c) "Upside-down" transformation of G_1 into G_2.

All isospectral pairs generated so far have an odd number of vertices, and this is the characteristic property of the presented procedure which cannot be overcome [8]. Nevertheless, it can produce coronoid IBGs with an even number of vertices (see fig. 8 and the explanation in the text). The most tempting question now is whether the conjecture in ref. [1] can also be disproved for (regular) benzenoids with an even number of vertices.

There is an attractive structural property of IBGs obtained by this procedure, namely, all of them can be depicted as being built from phenalene blocks, as shown in fig. 7(a). Any two adjacent blocks stick to each other exclusively in the way depicted in fig. 7(b): a convexity of one enters into a concavity of another. This requirement implies the same orientation of all present tiles. All benzenoids built in this way have an odd number of vertices, and this coincides with the noted property of the obtained IBGs. There is a relation between so-viewed isospectral mates which may be used as an amusing way for their construction. An example is shown in fig. 7(c): first, a BG must be built from phenalene tiles in the prescribed manner. Second, each block must be rotated in a place for 180°. This can be done in more equivalent ways and one of them is depicted in fig. 7(c). When the rotation is completed, phenalene tiles again stick tightly to each other and the obtained BG, if not also isomorphic, is isospectral to the starting one. This procedure can also be used to obtain coronoid IBGs, with an even or an odd number of vertices. In that

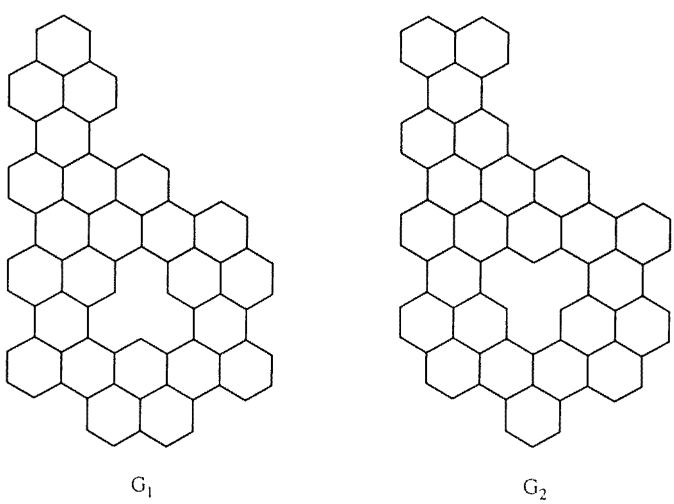

Fig. 8. The two coronoid IBGs built from phenalene tiles and mutually related by the "upside-down" transformation.

order, one has to build up a coronoid BG from phenalene tiles. Then, the "upside-down" transformation will produce its isospectral mate (which has yet to be checked on an isomorphism). An example of such a pair is shown in fig. 8.

It is not difficult to find out that each phenalene tile in G corresponds to a hexagon in $D(H'(G))$ and that their sticking scheme provides a perimeter of $D(H'(G))$ free of fissures, coves and fjords. A described "upside-down" transformation of a phenalene tiling is related to a transition from one colored $D(H'(G))$ to another one. Therefore, the last procedure is only a more appealing presentation of the previously described one.

Specific properties of the phenalene graph, useful for the construction of isospectral graphs, have already been observed and studied in ref. [9]. Further investigation in this direction, as well as a more formal formulation of the described procedure, is under way [6].

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References

[1] J. Cioslowski, J. Math. Chem. 6(1991)111.

[2] N. Trinajstić, *Chemical Graph Theory*, Vol. 1 (CRC Press, Boca Raton, 1983); I. Gutman and O.E. Polansky, *Mathematical Concepts in Organic Chemistry* (Springer, Berlin, 1986).

[3] I. Gutman and S.J. Cyvin, *Introduction to the Theory of Benzenoid Hydrocarbons* (Springer, Berlin, 1989).

[4] E. Heilbronner, MATCH (1979)105.

[5] F.T. Smith, J. Chem. Phys. 34(1979)105; A.T. Balaban and F. Harary, Tetrahedron 24(1968)2505.

[6] D. Babić and I. Gutman, in preparation.

[7] V. Grbović, S. Marković and I. Gutman, to be published.

[8] I. Gutman, private communication.

[9] W.C. Herndon and M.L. Ellzey, Jr., Tetrahedron 31(1975)99.