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Visualization of the resonance graphs of benzenoid graphs

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Abstract The vertex set of the resonance graph of a benzenoid graph G consists of 1-factors of G, two 1-factors being adjacent whenever their symmetric difference forms the edge set of a hexagon of G. We describe a computer program that generates and visualizes the resonance graphs of catacondensed benzenoid graphs.

1. INTRODUCTION

The drawing of complex molecules as well as the drawing of the related conceptual structures is a crucial element in many computer chemistry applications. Graph drawing algorithm is a method to produce graph drawing that meets some aesthetic criteria[1]. Since aesthetics frequently conflicts with each other, the most graph drawing algorithms set up a precedence relation among aesthetics. In order to establish a suitable precedence, it is often important to take into account the class of graphs to which a graph that needs to be drawn belongs. Specialized drawing algorithms then usually works better on the corresponding class of graphs than more general ones. Moreover, besides producing a more readable drawing, a tailor-made drawing algorithm can also illustrate the combinatorial properties of a graph.

Benzenoid graphs are defined as 2-connected subgraphs of the hexagonal lattice. A benzenoid graph G is *catacondensed* if any triple of hexagons of G has empty intersection, cf. Figure 1.

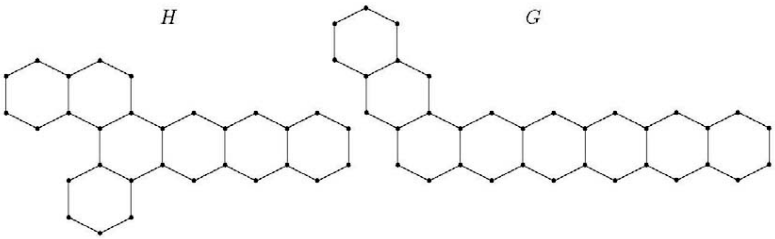

Figure 1. Two examples of catacondensed benzenoid graphs.

Catacondensed benzenoid graphs form a well studied class of graphs. Among many different topics studied on this class of graphs we briefly mention counting the number of Kekulè structures[17,18], the theory of elementary edge-cuts[9,11], the Schultz index (or molecular topological index, MTI)[3] and the coding problem of Kekulè structures[12]. For more information on benzenoid graphs and related concepts we refer to the book[8].

The concept of the resonance graph was brought out independently in mathematics (under the name Z-transformation graphs) by Zhang, Guo, and Chen[19] (see also[20, 21]) and in chemistry first by Gründler[6,7] and later by El-Basil[4, 5] as well as by Randić with co-workers[15, 16]. The concept appears to be very natural in chemistry. Some authors consider Kekulè structures as quantum - mechanical objects among which some (quantum - mechanical) interactions exist. In the case of benzenoid molecules the simplest model for such interactions is the following: if two Kekulè structures differ in the position of three double bonds, then they interact (by an unspecified, but constant amount); otherwise their interaction is neglected. Within this model the concept of the so-called resonance graph occurs naturally: The vertices of the resonance graph $R(G)$ of the benzenoid hydrocarbon B are the Kekulè structures of B; two vertices of $R(G)$ are adjacent if the corresponding Kekulè structures interact, that is if they differ in the position of just three double bonds.

In this paper we describe a computer program that generate and visualize the resonance graphs of benzenoid graphs. In the next section we give definitions and concepts needed in this paper. In particular we describe the decomposition theorem and the canonical coding of the resonance graphs of benzenoid graphs that play a crucial role in our drawing algorithm.

This algorithm is presented in Section 3, while the other functionalities of the program are given in Section 4.

2. MATHEMATICAL BACKGROUND

By a *graph* we mean a set $V(G)$ of vertices, together with a set $E(G)$ of edges. A graph is the *complete graph* K_n if any two of its distinct vertices are adjacent. A graph is the *path* P_n if it is isomorphic to a graph on n distinct vertices $v_1, v_2, \ldots, v_n$ and $n-1$ edges v_i, v_{i+1}, $1 \le i < n$.

A 1-factor (or perfect matching) of a graph G on n vertices is a selection of $n/2$ mutually independent edges of G. Only graphs with even number of vertices may have 1-factors, and then every vertex is the endpoint of exactly one of the selected edges. The fact that a Kekulè structure of a conjugated molecule is in a one – to - one correspondence with a 1-factor of the underlying molecular graph is well and long known. In the following considerations we shall, where appropriate, instead of "Kekulè structure" use the equivalent, but somewhat more precise, mathematical term "1-factor".

Let G be a benzenoid graph. Then the vertex set of the *resonance graph* $R(G)$ of G consists of the 1-factors of G, two 1-factors being adjacent whenever their symmetric difference forms the edge set of a hexagon of G. For instance, the construction of the resonance graph of the *linear chain* with four hexagons L_4 is presented in Figure 2. Note that it is straightforward to see that the resonance graph of the linear chain with h hexagons is isomorphic to the path on $h+1$ vertices. More formally: $R(L_h) = P_{h+1}$. We also set $R(K_2) = R(K_1) = K_1$.

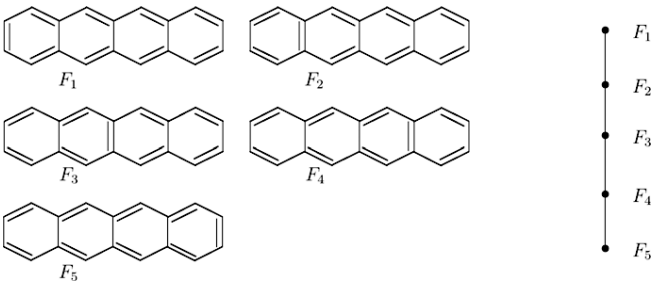

Figure 2. Linear chain L_4, 1-factors F_1, F_2, F_3, F_4, F_5 of L_4, and its resonance graph $R(L_4)$.

The *Cartesian product* $G\Box H$ of graphs G and H is the graph with the vertex set $V(G)\times V(H)$ and $(a,x)(b,y)\in E(G\Box H)$ whenever $ab\in E(G)$ and $x=y$, or, if $a=b$ and $xy\in E(H)$. In Figure 3 the Cartesian product of the path on 3 vertices P_3 and the path on 6 vertices P_6 is depicted.

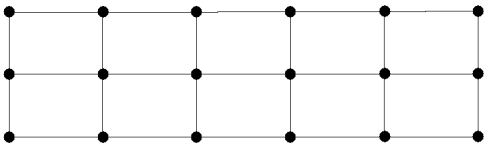

Figure 3. $P_3\Box P_6$

It is well known that the Cartesian product is associative, cf. Prop. 1.36 [10]. Hence the Cartesian product of graphs $G_1,G_2,\ldots,G_k$ can be written as $G_1\Box G_2\Box\cdots\Box G_k$. The vertex set of such a product is then the set of all k-tuples $(u_1,u_2,\ldots,u_k)$, where $u_i\in G_i$, while $(u_1,u_2,\ldots,u_k)$ is adjacent to $(v_1,v_2,\ldots,v_k)$ whenever there is an index j such that u_jv_j is an edge of G_j and $u_i=v_i$ for all $i\neq j$. The n*-cube* Q_n (or the n*-dimensional hypercube*) is the graph whose vertices are all binary words of length n, two words being adjacent whenever they differ in precisely one place. In other words, Q_n is just the Cartesian product of n copies of the complete graph on two vertices K_2.

For $u,v\in V(G)$, $d_G(u,v)$ or $d(u,v)$ denotes the length of a shortest path in G from u to v. If H is a subgraph of G, such that $d_H(u,v)=d_G(u,v)$ for all $u,v\in H$, then H is an isometric subgraph. Isometric subgraphs of hypercubes are called *partial cubes*.

Klavžar, Žigert and Brinkmann[14] proved that the resonance graph of a catacondensed benzenoid graph is a partial cube. In other words, the resonance graph $R(G)$ of a catacondensed benzenoid graph G with h hexagons can be isometrically embedded into the h-dimensional hypercube Q_h. Moreover, they showed an even stronger statement, namely that $R(G)$ is a median graph. This result turned out to be very useful, as it led to an algorithm

that assigns a unique and quite short binary code to every 1-factor of a catacondensed benzenoid graph[12].

For a subset X of vertices of a graph G, the subgraph of G induced by X is denoted by $G[X]$.

Let H be a fixed subgraph of a graph G, $H \subseteq G$. The *peripheral expansion* $\mathrm{pe}(G;H)$ of G with respect to H is the graph obtained from the disjoint union of G and an isomorphic copy of H, in which every vertex of the copy of H is joined by an edge with the corresponding vertex of $H \subseteq G$. Note that the ends of the newly introduced edges induce a subgraph of $\mathrm{pe}(G;H)$ isomorphic to $H \square K_2$. This concept is illustrated on Figure 4.

Let e be an edge of a hexagonal graph G. Then the *cut* C_e corresponding to e is the set of edges so that with every edge e' of C_e also the opposite edge with respect to a hexagon containing e' belongs to C_e.

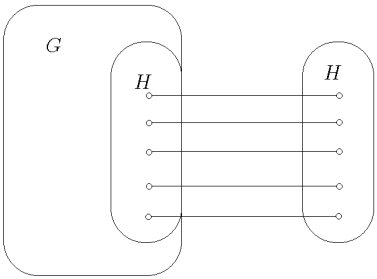

Figure 4. Peripheral expansion.

Let G be a catacondensed benzenoid graph and e an edge of G with ends of degree two. Let $e = e_0, e_1, \ldots, e_n$ be the edges of the cut C_e, and let $A_1 = A, A_2, \ldots, A_n$ be the corresponding hexagons. Let $e+$ and $e-$ be the edges of A_n incident to e_n, where $e+$ is the right edge looking from $e = e_0$ to e_n while $e-$ is the left edge. We say that $e+$ and $e-$ are *the right and the left turn-edge* of C_e, respectively. Remove now from G the hexagons $A_1, \ldots, A_n$, except the turn-edges $e+$ and $e-$. Then the remaining graph consists of two connected components G_{e+} and G_{e-}, where $e+ \in G_{e+}$ and $e- \in G_{e-}$. Note that any of G_{e+} and G_{e-} is

either a catacondensed benzenoid graph or a K_2. If G_{e+} is a catacondensed benzenoid graph, we repeat the described construction on G_{e+}, where the construction begins with $e+$. In this way we obtain two connected subgraph of G denoted G_{e++} and G_{e+-}. Similarly, if G_{e-} is a catacondensed benzenoid graph, then we repeat the construction on G_{e-}, starting with $e-$, to obtain connected subgraphs G_{e-+} and G_{e--}. In the case that $G_{e+} = K_2$ we set $G_{e++} = K_1$ and $G_{e+-} = K_1$, and if $G_{e-} = K_2$ we set $G_{e-+} = K_1$ and $G_{e--} = K_1$. These notations are illustrated in Figure 5.

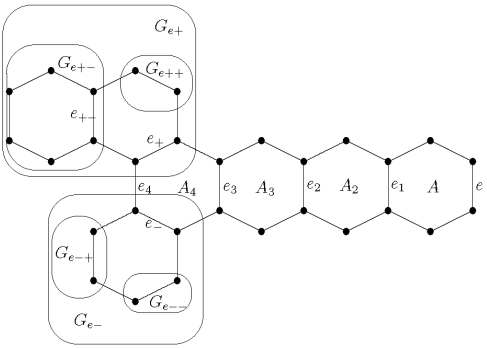

Figure 5. Recursive structure of a catacondensed benzenoid graph.

For a graph G, let $F(G)$ be the set of its 1-factors. If $e_1, e_2, \ldots, e_n$ are fixed edges of G, let $F(G; e_1, e_2, \ldots, e_n)$ denotes the set of those 1-factors of G that contain the fixed edges.

Klavžar, Vesel and Žigert [13] proved the following decomposition theorem. (The theorem is proved in the original form for more general class of catacondensed hexagonal graphs.)

Theorem 1 *Let G be a catacondensed benzenoid graph and e the edge with ends of degree two with $|C_e| = n+1$, where $n \geq 1$. Let $Y = R(G)[F(G;e)]$, $X = R(G)[F(G;e,e+,e-)]$, and X_1 the copy of X in Y_0 (the first Y-layer of $Y \square P_n$). Then*

$$R(G) = \mathrm{pe}(Y \square P_n; X_1).$$

Moreover,

- $Y = R(G_{e+}) \Box R(G_{e-})$ *and*
- $X_1 = X = R(G_{e++}) \Box R(G_{e+-}) \Box R(G_{e-+}) \Box R(G_{e--})$.

The decomposition theorem shows that the resonance graph of a catacondensed benzenoid graph G (with respect to the edge e with ends of degree two of G) is "almost" isomorphic to the Cartesian product of a smaller graph Y (defined as the Cartesian product of the resonance graphs of G_{e+} and G_{e-}) and a path on $n+1$ vertices.

For an example see the graph G from the right-hand side of Figure 1. Let e be the rightmost vertical edge of G. Then G_{e+} is isomorphic to L_2, while G_{e-}, G_{e++}, and G_{e+-} are isomorphic to K_2. Since $R(L_h) = P_{h+1}$, we have $R(G_{e+}) = P_3$, $R(G_{e-}) = R(G_{e++}) = R(G_{e+-}) = R(G_{e-+}) = R(G_{e--}) = K_1$. Therefore $Y = P_3 \Box K_1 = P_3$ and $X = K_1 \Box K_1 \Box K_1 \Box K_1 = K_1$. Since $|C_e| = 7$, we finally get $R(G) = \mathrm{pe}(P_3 \Box P_6; K_1)$. The resonance graph of G is depicted in Figure 6.

We have already mentioned the algorithm by means of which to every 1-factor of a catacondensed benzenoid graph (with h hexagons) a binary code of length h is assigned. By using the decomposition theorem Klavžar, Vesel and Žigert[13] designed an algorithm for the

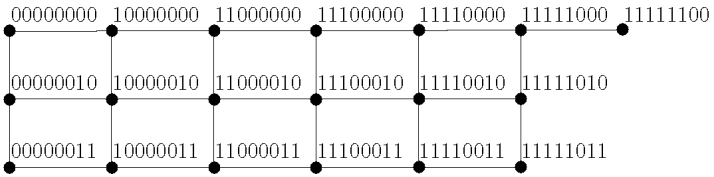

Figure 6. The resonance graph of G

canonical binary coding of 1-factors of a catacondensed benzenoid (hexagonal) graph. For a given edge e (with ends of degree two) the number of ones in the prefix of the canonical code corresponds to the index of the edge e_i. In particular, the code $1^i 0^{n-i} y_+ y_-$ of a vertex of $F(G; e_i)$, $0 \le i \le n-1$, (a vertex in a copy of Y in terms of the decomposition theorem) is composed of three parts: the prefix $1^i 0^{n-i}$ defines a position of a copy of Y in $Y \Box P_n$, while the substrings y_+ and y_- define a contribution of $R(G_{e+})$ and $R(G_{e-})$, respectively. The code of a vertex in $X = F(G; e_n)$ starts with n 1's. In addition, the rest of the digits are composed

of two substrings that start with 0: the first is the code of a vertex of $R(G_{e+})$ and the second is the code of a vertex of $R(G_{e-})$. More formally, if x is the code of a vertex of $F(G;e_n)$, then $x = 1^n ab$, where a (b) is a code of a vertex of $R(G_{e+})$ ($R(G_{e-})$) with 0 in the first place.

For the linear chain L_h with h hexagons (note that $R(L_{he+}) = R(L_{he-}) = K_1$) the canonical coding obviously returns

$$000\ldots00, 100\ldots00, 110\ldots00, \ldots, 111\ldots10, 111\ldots11.$$

The canonical binary coding of the resonance graph of the graph G from Figure 1 is little more involved. The code of a vertex in Y is of the form $1^i0^{6-i}y_+y_- = 1^i0^{6-i}y_+$ (note that $R(G_{e-}) = K_1$), where y_+ is a code of $R(G_{e+}) = R(L_3)$ from the set $\{00,10,11\}$. The codes of $R(G)$ are depicted in Figure 6.

The visualization algorithm is based on the following proposition.

Proposition 2 Let G be a catacondensed benzenoid graph with h hexagons and e the edge with ends of degree two with $|C_e| = n+1$, where $n \geq 1$. Then 1^i0^{h-i}, $0 \leq i \leq n$, is a canonical binary code of $R(G)$.

Proof. From the definition of the canonical binary coding follows that $0\ldots0$ is a canonical binary code of $R(G)$. Let x be a code of the i-th copy of Y. Then $x = 1^i0^{n-i}y_+y_-$, $0 \leq i < n$, where y_+ and y_- are arbitrary canonical codes of $R(G_{e+})$ and $R(G_{e-})$, respectively. Since both $R(G_{e+})$ and $R(G_{e-})$ contains a code with zeros in all places, the proposition follows for $i \leq n-1$.

Let now x be a code of X. Then $x = 1^n ab$, where a (b) is an arbitrary code of a vertex of $R(G_{e+})$ ($R(G_{e-})$) with 0 in the first place. Clearly, a (b) includes the code that contain zeros in all places and the proposition holds for $i = n$.

Hence we have finished the proof of the proposition. □

Note that the codes defined in Proposition 2 induce a path on n vertices that crosses all copies of Y as well as the subgraph X. This path will be called the *central path*.

3. DRAWING

A computer program that generates and visualizes the resonance graphs of catacondensed benzenoid graphs was written in Delphi Turbo Explorer programming environment. The program is equipped with a graphical user interface which allows the user to design a

catacondensed benzenoid graph as well as to control the visualization process using on-screen pull-down menus, icons, option boxes and other graphical devices. The program works on Windows computers and is available via the World Wide Web at http://www-mat.pfmb.uni-mb.si/personal/vesel/visual/visualHBG.html.

The typical run of the program sticks with the following steps.

1. Catacondensed benzenoid graph G is created by clicking the hexagons of the displayed hexagonal lattice (Figure 7).
2. An edge e (with ends of degree two) of G is chosen (Figure 8).
3. The codes of 1-factors of $R(G)$ are computed using the canonical binary coding.
4. The resonance graph $R(G)$ is drawn (see Figure 9).

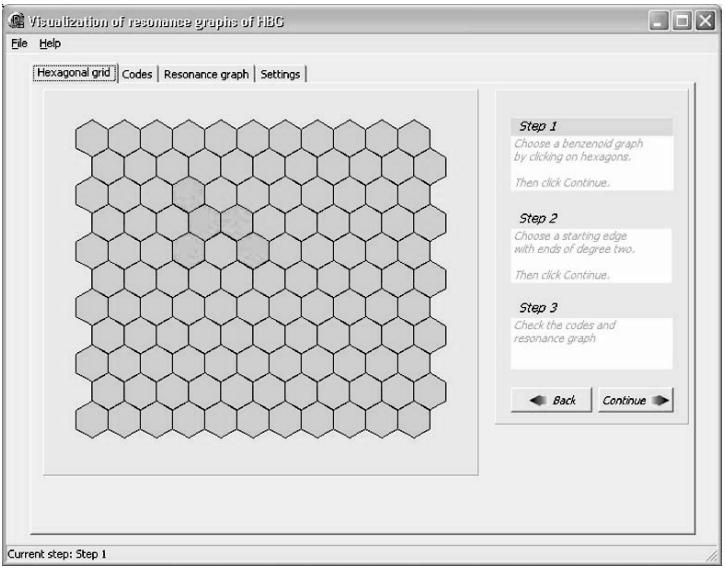

Figure 7. Creating catacondensed benzenoid graph G

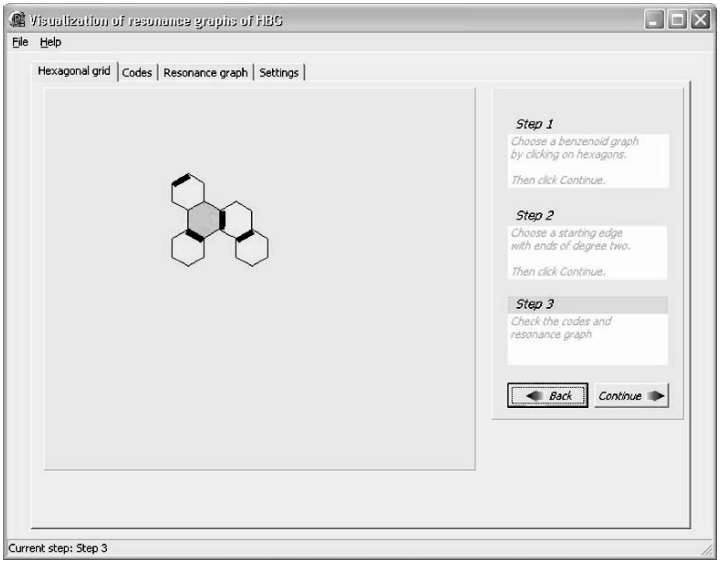

Figure 8. An edge e of G is chosen

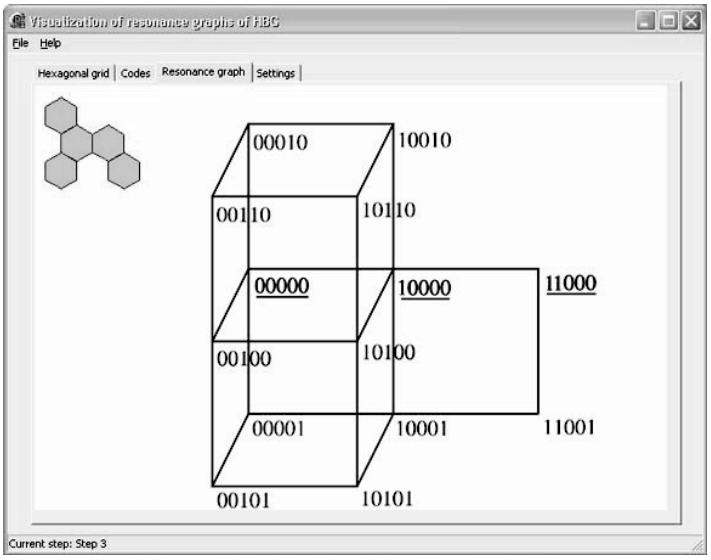

Figure 9. The resonance graph $R(G)$ is drawn

The following remarks are in order:

- When the edge e is chosen, components G_{e+}, G_{e-}, G_{e++}, and G_{e-+} are marked in the drawing of G.
- The canonical codes of the resonance graph are displayed at tab Codes as is shown on Figure 10.
- The canonical codes are displayed also in the final drawing of the resonance graph.

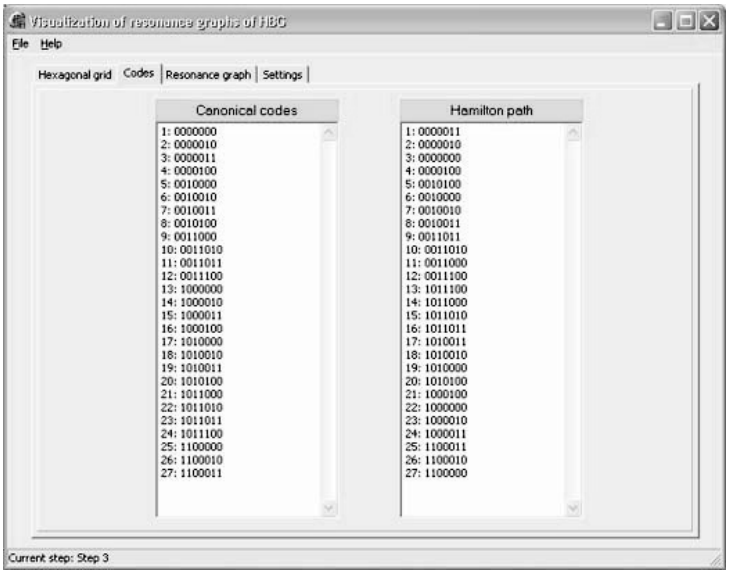

Figure 10. The canonical codes and the Hamilton path

The heart of the program is the procedure that draws the resonance graphs of catacondensed benzenoid graph. The procedure uses the benefits of the decomposition theorem as well as of the canonical binary coding. As we have already seen, the decomposition theorem shows that the resonance graph of a catacondensed benzenoid graph G (with respect to an edge e of G) is almost isomorphic to the Cartesian product of a certain smaller graph Y and a path on $n+1$ vertices. More precisely, the resonance graphs of a catacondensed benzenoid graph compose n copies of Y and a subgraph X of Y. The canonical coding assigns a binary string to every 1-factor of a catacondensed benzenoid graph. Every string contains a prefix 11…100…0 of

length n, where the number of ones corresponds to the position of a copy of Y in $R(G)$. In particular, the 1-factors of the first copy of Y receive the prefix $00\ldots0$, whilst the 1-factors of X receive the prefix 11…1.

The drawing is based on the representation of $R(G)$ in R^3. In other words, we defined a mapping from $V(G)$ to R^3. The main idea of the mapping is to assign the vertices of each copy of Y as well as the vertices of X to a separate plane. The following algorithm describes the main steps of the idea presented above.

Procedure Draw($R(G)$);

1. Draw Central Path.
2. **for** all vertices v of $R(G)$ **do**
   2.1. **for** all unvisited vertices u adjacent to v **do**
      2.1.1 **if** the number of visited vertices adjacent to u is at least 2 **then**
         Determine coordinates of u using the parallelogram rule
      else
         Determine coordinates of u using the coordinate table
      2.1.2 **if** coordinates do not satisfy constraints **then**
         Visualization: = unsuccessful.
         Exit Draw.
3. Visualization:= successful.

The procedure Draw first calls an auxiliary procedure Draw Central Path. The result of Draw Central Path is a straight horizontal or inclined (depending on the complexity of the graph) line, which indicates the final look of $R(G)$. Furthermore, the distances between planes to which vertices of X and consecutive copies of Y are mapped are also computed. Particularly, Draw Central Path visualizes the vertices and the edges of the central path together with the corresponding codes. The codes of the central line are depicted bold as can we see in Figure 12. Since from Prop. 2 follows that the central path crosses all copies of Y (as well as the subgraph X), a vertex of the central path represents a starting point for the visualization of the corresponding copy of Y (as well as of X).

In the main **for** loop of the procedure all vertices of $R(G)$ are examined. The order of the vertices depends on the Central Path, i.e. the vertices of the Central Path are considered first, then their neighbors etc. The procedure for every vertex of a graph searches for its adjacent unvisited vertices. An adjacent unvisited vertex u is checked, whether it has at least two already visited neighbors. If it does, then Step 2.1.1. is executed and the coordinates of u are

determined by the parallelogram rule. The situation is illustrated on Figure 11 where a and b denote some already visited vertices adjacent to u while c denotes the common neighbor of a and b.

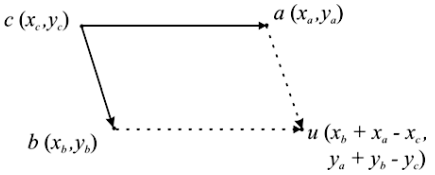

Figure 11. Coordinates of u

If u does not have at least two visited adjacent vertices, then the coordinates are determined using the *directions table* (see Table 1), which contains all possible coordinates of the vertex u relative to the vertex v. The coordinates depend on the value denoted *edge* which is set to 80 pixels by default and can be altered by the user. Coordinates of u are determined in the order given by directions table, thus changing the order in the table results in changed representation of $R(G)$.

In Step 2.1.2 the algorithm checks, whether computed coordinates satisfy some obvious constraints. In other word, the algorithms determines, if the position of the current vertex overlaps some other vertex or lies on some already determined edge of $R(G)$. If this happens for all coordinates computed in Step 2.1.1, the attempt to visualize $R(G)$ fails.

The procedure is successful, when appropriate coordinates for all vertices of $R(G)$ are found.

direction	x - coordinate	y - coordinate
1	$x_v + edge$	y_v
2	x_v	$y_v - edge$
3	$x_v - edge$	y_v
4	x_v	$y_v + edge$
5	$x_v + (edge/4)$	$y_v - (edge/4)$
6	$x_v - (edge/4)$	$y_v - (edge/4)$
7	$x_v - (edge/4)$	$y_v + (edge/4)$
8	$x_v + (edge/4)$	$y_v + (edge/4)$

Table 1. Directions table

4. OTHER FUNCTIONALITIES OF THE PROGRAM

Hamilton path

Chen and Zhang[2] proved that the resonance graph of a catacondensed benzenoid graph has a Hamilton path. An algorithm that for a (slightly) more general class of catacondensed hexagonal graphs returns such a path is presented by Klavžar, Vesel and Žigert [13]. The algorithm intrinsically uses the canonical coding in order to list the vertices in a Hamilton path. The sequence of labels that composes a Hamilton path in the resonance graph of a given graph is displayed on tab Codes (see Figure 10).

Saving and loading a graph

The program saves resonance graphs in various graphic formats, e.g. eps, jpeg and bmp. It is also possible to save canonical codes of the graph in a plain text file for a later use. The user can also load canonical codes from a text file and the corresponding graph is then drawn and presented on tab Resonance graph (see Figure 12).

Customization of the drawn resonance graph

If the user wants to change the resonance graph in order to try some other aspect of the visualization, he/she can pick the vertex (with the left mouse button) and move it to the desired location. The user can also move simultaneously the whole array of corresponding vertices of all copies of Y (the concept is illustrated on Figure 13). It is also possible to turn on the grid of lines in predetermined spacing, which are meant as visual aid for the user. Some other options regarding customization of the drawing are described bellow.

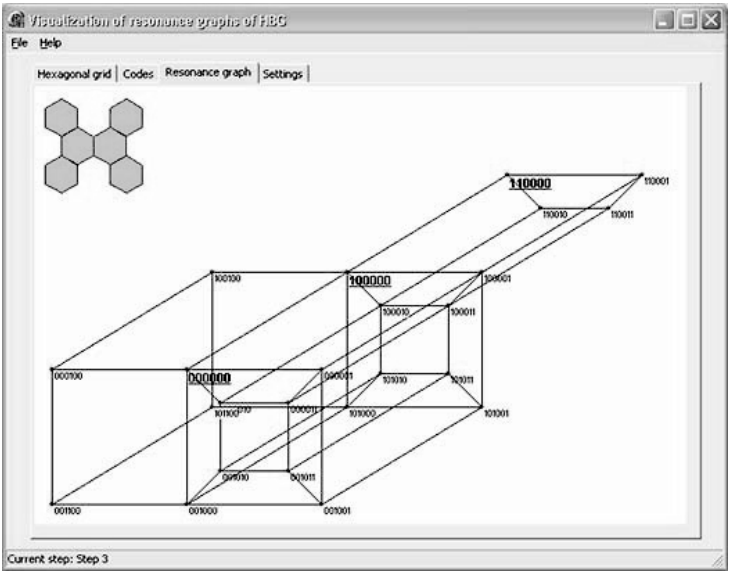

Figure 12. Example of the resonance graph

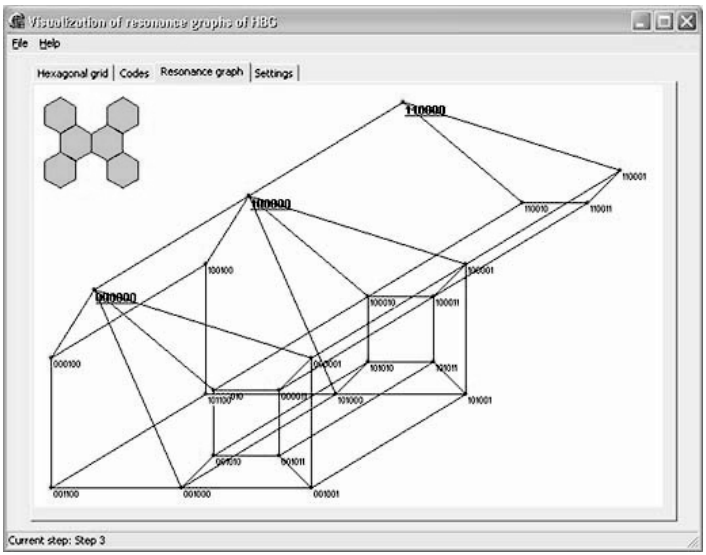

Figure 13. Moving the array of vertices

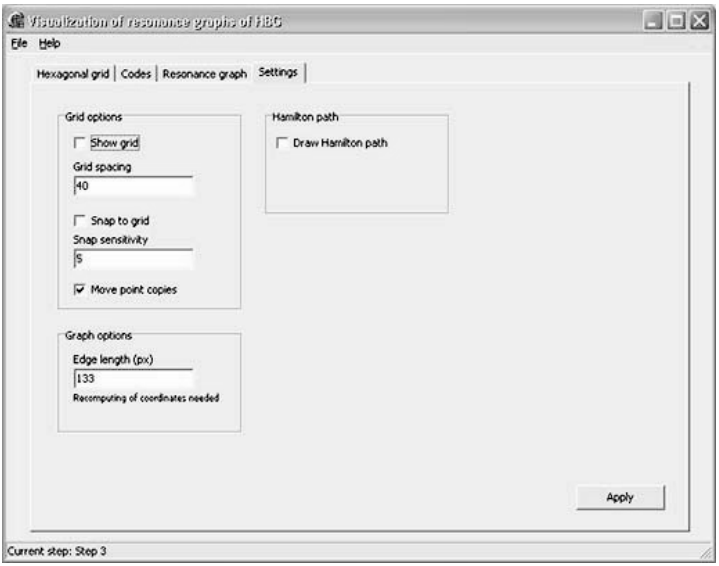

Figure 14. Settings

Options

Various options for controlling the process of drawing the resonance graphs are available in tab Settings (see Figure 14).

- Length of edges: the user can change the length of the edges of the central path. The other edges of the graph are then also proportionally altered.
- Draw Hamilton path: if checked, the edges of the Hamilton path are inscribed in the resonance graph with green color. The starting and ending vertex are also marked.
- Grid options: grid options were designed to add visual aid for the user when moving vertices in the resonance graph
    - Show grid: turns on/off the grid
    - Grid spacing: determines the vertical and horizontal whitespace between the lines in the grid
    - Snap to grid: if checked, junctions in the grid become magnetic i.e. they attract vertices to them when user moves them

- Snap sensitivity: determines the range where vertices are still attracted to the grid junction
- Move point copies: if checked, the corresponding vertices of the vertex held by the mouse in all copies of Y are also moved.

More detailed instructions on how to use the program are in the program help and on the website[22].

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