ELSEVIER

Discrete Applied Mathematics 118 (2002) 209–222

DISCRETE APPLIED MATHEMATICS

Boundary uniqueness of fusenes

Xiaofeng Guo[a], Pierre Hansen[b,*], Maolin Zheng[c]

[a] *Institute of Mathematics and Physics, Xinjiang University, Wulumuqi, People's Republic of China*
[b] *GERAD, École des Hautes Études Commerciales, Ecole Polytechnique Montréal, 5255 Ave. Decelles, Montréal, Que. Canada H3T1V6*
[c] *Lexis-Nexis, Dayton, Ohio, USA*

Received 1 October 1999; received in revised form 4 April 2000; accepted 15 January 2001

Abstract

It is shown that a geometrically planar fusene is uniquely determined by its boundary edge code. Surprisingly, the same conclusion is not true in general but holds for geometrically planar and non-planar fusenes with at most 25 hexagons, except for two particular cases. In addition, it is proved that two fusenes with the same boundary edge code have the same number of hexagons.

Keywords: Chemical graph; Fusene; Code; Uniqueness

1. Introduction

Hexagonal systems or geometrically planar polyhexes are extensively studied in the literature of benzenoid hydrocarbons [2–5,10,13,14,20,22]. A polyhex consists of congruent regular hexagons in which any two hexagons are either disjoint or share a single edge and any vertex has degree 2 or 3. By convention, a polyhex is geometrically drawn in the plane such that some of its edges are vertical and no two adjacent hexagons are folded on each other. A *boundary edge* of a polyhex H is an edge which belongs to only one hexagon. A *boundary vertex* is an end vertex of a boundary edge. A *boundary hexagon* is a hexagon which contains at least one boundary edge. The *boundary* $B(H)$ consists of all the boundary edges. If $B(H)$ is a circuit, then H is simply connected and called a *fusene*. If a fusene is not geometrically planar, it is called a *helicene*. Let $V(H)$ and $h(H)$ denote the set of vertices and the number of hexagons of H, respectively.

* Corresponding author. Fax: +1-514-340-5665.
E-mail address: pierreh@crt.umontreal.ca (P. Hansen).

0166-218X/02/$ - see front matter
PII: S0166-218X(01)00180-9

Polyhexes correspond to known or unknown polycyclic hydrocarbons with only six-membered rings. A lot of work has been devoted to enumerate polyhexes with a given number of hexagons or particular subsets thereof (for example, planar polyhexes, polyhexes possessing certain symmetries) [2,6,15,17,18,7,21]. Recently, enumeration of fusenes was extended to 20 hexagons [8]. This result was achieved by using the *boundary-edges* (BE) *code* [11], and *reverse search* [1]. Note that in this case reverse search is equivalent to *orderly generation* [9,16,19]. The generation is guaranteed by the following claim: a fusene with not more than 21 hexagons is uniquely determined by its BE code. Is this still true in general? In other words, is a fusene uniquely determined by its boundary? For geometrically planar fusenes, the answer is positive. The proof will be given later. Surprisingly, the same result does not hold for all fusenes. However, we prove that it holds for fusenes of at most 25 hexagons with two exceptions. Even if the answer to the above question is not true in general, the following claim is valid: two fusenes have the same number of hexagons if they have the same boundary edge code.

2. BE code and $h(H)$

We first describe the BE code [11]. For fusenes, it is equivalent to the PC-2 code [12] and obtained as follows: beginning at any boundary vertex of degree 3, which thus belongs to 2 hexagons, follow the boundary of the polyhex noting by a digit the number of edges for each successive hexagon encountered. Observe that the same hexagon may appear up to three times on the boundary, and hence may contribute up to 3 digits to the code. Then apply, if needed, a circular shift and/or an order reversal to the code to make it lexicographically maximum. Construction of the BE code of a polyhex is illustrated on Fig. 1. Note that the BE code may be obtained in several ways in case of symmetry of the polyhex.

Let H_1 and H_2 be two fusenes. An *isomorphism* f from H_1 to H_2 is a one-to-one mapping from $V(H_1)$ to $V(H_2)$ which maps only adjacent vertices to adjacent vertices. If $H_1 = H_2$, then f is called a *symmetry mapping* or an *automorphism*. It is said that H_1 is *isomorphic* to H_2 if there is an isomorphism from H_1 to H_2.

A *boundary symmetry mapping* g from H_1 to H_2 is a one-to-one mapping from boundary vertices of H_1 to boundary vertices of H_2 such that (i) a vertex v and its image $g(v)$ have the same degree, and (ii) two vertices are adjacent in $B(H_1)$ if and only if their images are adjacent in $B(H_2)$. The inverse g^- of g is a boundary symmetry mapping from H_2 to H_1 too. An edge e is mapped onto an edge e' by g if the vertices of e are mapped onto the vertices of e'. Let $g(e)$ denote e'. A hexagon s is mapped onto a hexagon s' by g if at least one edge of s is mapped onto an edge of s'. By the definition, s may be mapped onto several hexagons. Let $g(s)$ denote the set of hexagons which s is mapped onto. Furthermore, if N is a set of boundary vertices, then let $g(N)$ denote the set of the images of the vertices in N.

Fig. 2 shows two helicenes with the same BE but they are not isomorphic.

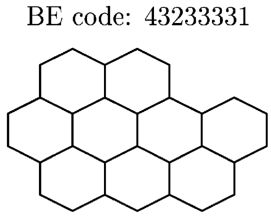

Fig. 1. A geometrically planar fusene and its BE code.

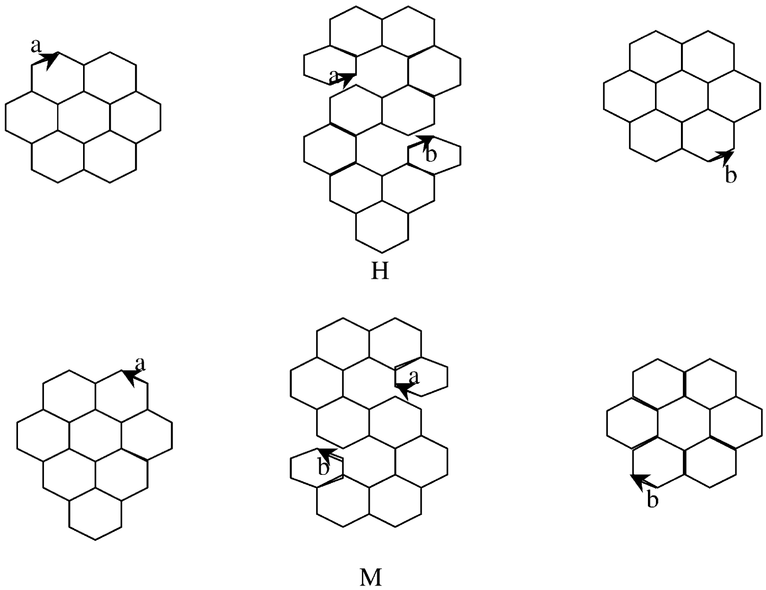

Fig. 2. Non-isomorphic helicenes with same BE code. The helicenes H and M in the figure should be viewed as follows: H is the helicene obtained by identifying edge a together with its direction in the left fusene to the edge a in the middle one, and the edge b with its direction in the right fusene to the edge b in the middle one; M is obtained in a similar way.

By definition, for a boundary symmetry mapping we have the following:

Theorem 1. *Two fusenes H_1 and H_2 have the same BE code if and only if there is a boundary symmetry mapping from H_1 to H_2.*

Now we prove that two fusenes have the same number of hexagons if they have the same BE code.

Theorem 2. *If H_1 and H_2 have the same BE, then $h(H_1) = h(H_2)$.*

Proof. Let f be a boundary symmetry mapping from H_1 to H_2. Since H_1 and H_2 have the same BE code, we can draw H_1 and H_2 in the plane such that their boundaries are identical, or in other words, for any boundary edge e, $f(e)$ will occupy the same position as e does. We also assume some of their edges are vertical. In addition, any two parallel vertical edges of the same hexagon have distance one. Note that this drawing may result in some non-adjacent hexagons of H_1 or H_2 overlapping.

For each vertical edge e, let $x(e)$ denote the x-coordinate of the points on e.

Consider the polyhex G_L consisting of all hexagons of H_1 on the same horizontal level L. Then each connected component of G_L is a fusene (actually a hexagon chain). Let $G_L^1, G_L^2, \ldots, G_L^m$ be the connected components of G_L. Let e_l^i and e_r^i be the leftmost edge and the rightmost edge of G_L^i, respectively. Then $h(G_L^i) = x(e_r^i) - x(e_l^i)$ and therefore

$$h(G_L) = \sum_{i=1}^{m} h(G_L^i) = \sum_{i=1}^{m} (x(e_r^i) - x(e_l^i)) = \sum_{i=1}^{m} x(e_r^i) - \sum_{i=1}^{m} x(e_l^i).$$

The hexagons on level L and belonging to H_2 also form a polyhex G_L'. Let W_L^i $(i = 1, \ldots, k)$ be the connected components of G_L'. Note that the vertical boundary edges of H_2 on level L are the images of the vertical boundary edges of H_1 on level L. Thus $k = m$. Let g_l^i and g_r^i be the leftmost edge and the rightmost edge of W_L^i, respectively. By the same reasoning as the above,

$$h(G_L') = \sum_{i=1}^{m} h(W_L^i) = \sum_{i=1}^{m} (x(g_r^i) - x(g_l^i)) = \sum_{i=1}^{m} x(g_r^i) - \sum_{i=1}^{m} x(g_l^i).$$

Also by the way H_1 and H_2 are drawn, we have that e is the leftmost (the rightmost) edge of a connected component of G_L if and only if $f(e)$ is the leftmost (the rightmost) edge of a connected component of G_L'. Thus

$$\begin{aligned}
h(G_L) &= \sum_{i=1}^{m} h(G_L^i) \\
&= \sum_{i=1}^{m} (x(e_r^i) - x(e_l^i)) \\
&= \sum_{i=1}^{m} x(e_r^i) - \sum_{i=1}^{m} x(e_l^i) \\
&= \sum_{i=1}^{m} x(f(e_r^i)) - \sum_{i=1}^{m} x(f(e_l^i)) \\
&= \sum_{i=1}^{m} x(g_r^i) - \sum_{i=1}^{m} x(g_l^i) \\
&= h(G_L').
\end{aligned}$$

From this, it can easily be shown that $h(H_1) = h(H_2)$. $\square$

3. Boundary uniqueness

In this section, we will show that two fusenes with the same BE are isomorphic if they have at most 25 hexagons, with two exceptions. In order to accomplish this, a few definitions and lemmas are needed.

Let H be a fusene and s a hexagon. Let $H-s$ denote the polyhex consisting of all hexagons of H other than s. Throughout the remainder of the paper, we assume that $h(H)>1$. A boundary hexagon s is *removable* if $H-s$ is a fusene (it may be planar), otherwise it is *non-removable*. A boundary hexagon is of *i*-type if it contributes a digit i to the BE code (where $i=1,2,\ldots,5$). By definition, a 3-type hexagon might be a 1-type hexagon as well.

Lemma 1. *Let H be a fusene and s a boundary hexagon. Then, s is removable if and only if it contributes only one digit to the BE code of H.*

Proof. s is removable if and only if $H-s$ is a fusene. $H-s$ is a fusene if and only if $H-s$ is connected. $H-s$ is connected if and only if $s\cap B(H)$ is connected, i.e., s contributes only one digit to the BE code of H. □

Corollary 1. *A 4-type or 5-type hexagon of a fusene is removable.*

Let H be a fusene and s a non-removable hexagon. Then $H-s$ is disconnected and each of its components is a fusene. By noting that s contributes at most 3 digits to the BE of H, $H-s$ has at most 3 connected components. The union of a connected component of $H-s$ and s, denoted by $H*s$, is a fusene. For $H*s$ we have the following lemma:

Lemma 2. *$B(H*s)-s$ is contained in $B(H)$ and s is removable in $H*s$. A non-removable hexagon of $H*s$ is non-removable in H. Each removable hexagon of $H*s$, except s, is removable in H.*

Proof. By the way $H*s$ is defined, s is removable in $H*s$ and $B(H*s)-s$ is contained in $B(H)$. Let h be a boundary hexagon of $H*s$ other than s. Then $h\cap B(H)=h\cap B(H*s)$. Thus h contributes the same number of digits to the BE code of H as to the BE code of $H*s$. By Lemma 1, h is removable in H if and only if it is removable in $H*s$. □

Corollary 2. *A boundary hexagon of $H*s$ which is not s has the same type both in H and $H*s$.*

A sub-fusene L of H is called a *leaf sub-fusene* (*LSF*) if it has no non-removable hexagons and it is the union of a non-removable hexagon s of H and a connected component of $H-s$ (s is called the ear of L). Let L be a LSF of H. By the above definition and Lemma 2, we have:

Lemma 3. (1) *A boundary edge of L is also a boundary edge of H if it does not belong to the ear.* (2) *Each boundary hexagon of L except the ear is also a boundary hexagon of H.* (3) *Each boundary hexagon of L except for the ear is removable in H.* (4) *The ear is removable in L but not in H.*

Lemma 4. *A fusene H with a non-removable hexagon has at least two LSFs.*

Proof. We prove the lemma by induction on $h(H)$. Let s be a non-removable hexagon. Then $H-s$ is disconnected and each of its connected components is a fusene. Let H_1 and H_2 be two sub-fusenes of H such that each of them is the union of s and a connected component of $H-s$. Now we show that each of H_1 and H_2 contains a LSF of H. Therefore the lemma is true. If H_1 has no non-removable hexagons, then it is a LSF of H. Otherwise, it has a non-removable hexagon which is also non-removable in H by Lemma 2. Since H_1 is smaller than H, by the induction hypothesis, it has at least two LSFs. Let G_1 and G_2 be two of LSFs of H_1. By Lemma 2 each boundary hexagon of $G_i (i=1,2)$ is a boundary hexagon of H_1 and therefore a boundary hexagon of H. By noting that s is removable in H_1, one of G_1 and G_2, say G_1, does not contain s. Let r be the ear of G_1. Since r is non-removable in G_1, it is non-removable in H_1 and thus in H. Let U be the connected component of H_1-r such that $G_1=U\cup r$. By the definition of H_1, U is also a connected component of $H-r$. Thus G_1 is a LSF of H. By the same reasoning, H_2 also contributes a LFS to H. The proof is completed. □

By the above lemma we have:

Corollary 3. *A fusene H with more than one hexagon has at least* 2 *removable hexagons.*

Proof. If every hexagon of H is removable then the lemma is valid. Otherwise by Lemma 4, H has two LFSs. By Lemma 3, each of them contains a removable hexagon of H. □

Lemma 5. *Let H be a fusene with some non-removable hexagons and no* 4- *and* 5-*type hexagons. Let L be a LSF of H. Then in L, the ear is* 3-, *or* 4-, *or* 5-*type and every other boundary hexagon of L is* 1-, *or* 2-, *or* 3-*type*.

Proof. By Corollary 1, each boundary hexagon of L other than the ear has the same type both in H and L. Therefore, it is not a 4- or 5-type hexagon. Since the ear is not removable in H, one can check that it cannot be 1,2-type in L. The proof is completed. □

The four fusenes in Fig. 3 are defined as a crown, a double-crown, a crown-plus and a double-crown-minus.

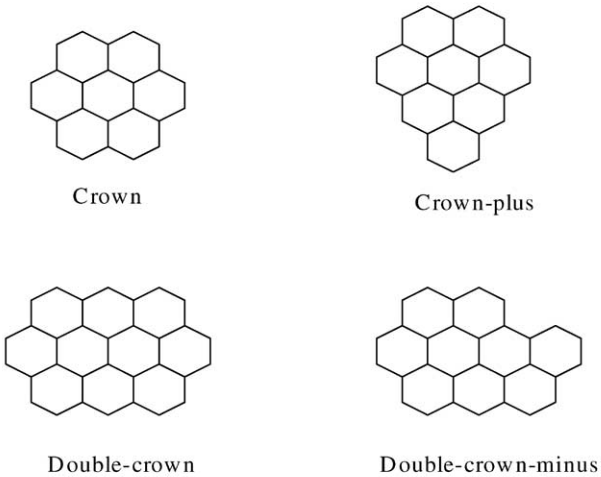

Fig. 3. Crown, double-crown, crown-plus and double-crown-minus.

Lemma 6. *Let H be a fusene which has no* 4-*type*, 5-*type and non-removable hexagons. Then* $h(H)$ *is* 7 *or greater than or equal to* 10. *If* $h(H)$ *is* 7, *then* H *is a crown. If* $h(H)$ *is* 10, *then* H *is a double-crown. Moreover*, *it has at least* 6 *hexagons of* 3-*type*.

Proof. The hexagons of H on the topmost row together form a polyhex H^{top} (it may not be connected). Let L_1 be a connected component of H^{top}. Then L_1 has at least 2 hexagons (otherwise, H will have a 4- or 5-type hexagon). Let L_2 be the polyhex consisting of the hexagons adjacent to and below the hexagons of L_1. First, L_2 is not empty (otherwise, H is a hexagonal chain and has two 5-type hexagons). Second, L_2 must be connected (otherwise H has a non-removable hexagon). Third, L_2 has more hexagons than L_1 (otherwise, it can be checked easily that H has a 4- or 5-type hexagon). Let L_3 be the polyhex consisting of the hexagons which are adjacent to and below the hexagons of L_2. Again, L_3 is not empty (otherwise, H has a 4- or 5-type hexagon). If there is a connected component of L_3 which has only one hexagon, then this hexagon is a non-removable or 4- or 5-type hexagon. This contradicts the assumption. Thus each component of L_3 has at least 2 hexagons. By the above conclusions, we have that $h(H) \geqslant 7$. Now consider the following two cases:

(a) All hexagons of H are on 3 different levels. Let H_{low} be the polyhex consisting of the hexagons at the bottom level. By the above proof, each connected component of H^{top} and H_{low} has at least two hexagons and L_2 has at least three hexagons. If both of H^{top} and H_{low} are disconnected, then $h(H) \geqslant 11$. Assume that $h(H) \leqslant 10$. Then at least one of H^{top} and H_{low} is connected.

Without loss of generality, let H^{top} be connected. Then $L_1 = H^{\mathrm{top}}$, and L_2 contains all the hexagons on the middle level. If H_{low} is not connected, then it has at least 4 hexagons. Therefore, L_2 has at least 6 hexagons (for H has no 4- or 5-type hexagons).

Thus $h(H) \geqslant 12$. So H_{low} is connected. Also note by the previous argument that $h(L_2) > h(H^{\mathrm{top}})$ and $h(L_2) > h(H_{\mathrm{low}})$. If $h(L_2) = 3$, H is a crown. If $h(L_2) = 4$, then $h(H^{\mathrm{top}}) = h(H_{\mathrm{low}}) = 3$. Thus H is a double-crown and $h(H) = 10$.

(b) All hexagons of H are on at least 4 levels. Then consider the hexagons on the lowest level and the second lowest level. By the same reasoning as for showing that L_1 and L_2 have at least 5 hexagons, the number of hexagons on the two levels is at least 5. So $h(H)$ is at least 10. If $h(H) = 10$, then the numbers of hexagons on these 4 levels will be 2,3,3,2. Thus H is a double-crown.

Note that on the highest level, there are at least 2 hexagons of 3-type. The same is true for the lowest level. Also the leftmost and rightmost hexagons are of 3-type. Therefore H has at least 6 hexagons of 3-type. The proof is completed. □

Lemma 7. *Let H be a fusene. Assume that H has no* 5-*type hexagons and has one* 4-*type hexagon. Each boundary hexagon is removable. Then* $h(H) \geqslant 8$. *If* $h(H) = 8$, *H is a crown-plus. If* $h(H) = 9$, *then H is the double-crown-minus. Moreover, H has at least* 4 *hexagons of* 3-*type.*

Proof. We prove the lemma by induction on $h(H)$. Let H' be the subpolyhex of H consisting of all hexagons except for the only 4-type hexagon. Then H' has at most one 4-type hexagon and no 5-type hexagons. Since H has no non-removable hexagon, H' is a fusene. One can check easily that each boundary hexagon of H' contributes only one digit to its BE code. By Lemma 1, H' has no non-removable hexagon.

If H' has no 4- or 5-type hexagons, by Lemma 6, $h(H') \geqslant 7$. If H' has one 4-type hexagon, then by induction, $h(H') \geqslant 8$. In both cases, $h(H) \geqslant 8$. If $h(H) = 8$, then H' satisfies the condition of Lemma 6. H' is a crown and thus H is a crown-plus. If $h(H) = 9$, then $h(H') = 8$ and H' satisfies the condition of the lemma. By induction, H' is a crown-plus. From this we have that H is a double-crown-minus.

For showing that H has at least 4 hexagons of 3-type, we draw H on the plane so that the only 4-type hexagon is lower than its adjacent hexagons and some of its edges are vertical. Then on the highest level, there will be at least 2 hexagons of 3-type. Consider the leftmost and the rightmost hexagons. They are also 3-type. Thus H has at least 4 3-type hexagons. □

An *SBE* pair (H_1, H_2) is a pair of fusenes having the same BE code (here H_1 may be equal to H_2). The pair is *irreducible* if there is a boundary symmetry mapping from H_1 to H_2 which maps each removable hexagon onto a non-removable hexagon. Otherwise, the pair is *reducible*. In Fig. 2, the two fusenes form a reducible *SBE* pair.

For an irreducible SBE pair of fusenes, we have the following lemmas:

Lemma 8. *If* (H, M) *is an irreducible SBE pair*, *then each of H and M has non-removable hexagons.*

Proof. Let f be a symmetry mapping from H to M which maps each removable hexagon of H to a non-removable hexagon of M. By Corollary 3, each M and H

has at least 2 removable hexagons. These removable hexagons in H (M) are mapped onto non-removable hexagons under f (f^-). Thus each of H and M has at least one non-removable hexagon. □

Lemma 9. *Let (H,M) be an irreducible SBE pair, then H and M have no* 4- *and* 5-*type hexagons. Moreover, a LSF of M or H has at least* 7 *hexagons, no* 5-*type hexagon and the ear is the only hexagon which may be* 4-*type in the LSF.*

Proof. Note that under any boundary symmetry mapping from H to M, a boundary hexagon and its image have the same type. If H has a 4- or 5-type hexagon s, then it will be mapped onto a 4- or 5-type hexagon of M under any boundary symmetry mapping from H to M. Thus s and its image are removable. This contradicts that (H,M) is irreducible. By Lemma 8, both H and M have non-removable hexagons. By Lemma 4, they have LSFs. Let L be a LSF of H. Since H has no 4- or 5-type hexagons, by Lemma 5 L has at most one 4- or 5-type hexagon which is the ear. If L has no 4- and 5-type hexagons, by Lemma 6 $h(L) \geqslant 7$. If L has one 4-type hexagon, by Lemma 7, $h(L) \geqslant 8$. The remaining case is that L has a 5-type hexagon. By Lemma 5, it is the ear. Since L does not have non-removable hexagons and its ear is 5-type, L has only 2 hexagons. Then L has one more 5-type hexagon which is also 5-type in H. This is a contradiction. The above proof is also valid for M. So each of H and M has at least 7 hexagons. □

Lemma 10. *Let (H,M) be an irreducible SBE pair of fusenes. Then $h(H)=h(M) \geqslant$ 24. If $h(H) = 24$, then H and M are the fusenes shown in Fig.* 4 *and they are isomorphic.*

Proof. Since (H,M) is irreducible, there is a boundary symmetry mapping, f, from H to M which maps each removable hexagon of H onto a non-removable hexagon of M. Then the inverse f^- of f is a boundary symmetry mapping from M to H which maps each removable hexagon of M onto a non-removable hexagon of H. The above fact will be used explicitly or implicitly in the proof.

By Lemma 8, each of H and M has non-removable hexagons. By Lemma 4, let B_H^1 and B_H^2 be two LSFs of H and B_M^1 and B_M^2 two LSFs of M. Let S_M^i (S_H^i) be the polyhex consisting of the boundary hexagons of B_M^i (B_H^i) excluding the ear ($i=1,2$). Let $f^-(S_M^i)$ denote the polyhex of H consisting of the hexagons onto which the hexagons of S_M^i are mapped under f^- ($i=1,2$). Roughly speaking, $f^-(S_M^i)$ is the image of S_M^i under f^-. By Lemma 9, B_H^i and B_M^i ($i=1,2$) have no 5-type hexagons in themselves.

By Theorem 2, $h(H)=h(M)$.

We have the following cases:

Case 1. One of B_M^i ($i=1,2$) has at least 10 hexagons. By Lemma 9, both of them together have at least 17 hexagons. By Lemmas 6 and 7, B_H^1 and B_H^2 have at least 8 hexagons which are 3-type and removable in H and are mapped by f onto

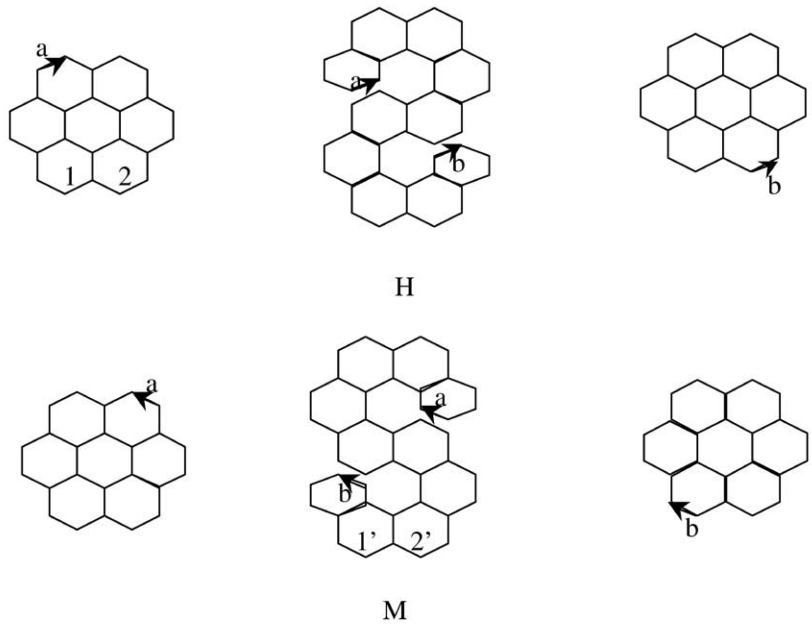

Fig. 4. An irreducible SBE pair with a boundary symmetry mapping f such that $f(1) = 1'$ and $f(2) = 2'$. H and M should be viewed in a similar way as in Fig. 2.

non-removable 3-type hexagons of M. Note that the ears of B_M^1 and B_M^2 are not 3-type hexagons in M for they are non-removable in M. Thus the eight 3-type non-removable hexagons of M do not belong to B_M^1 and B_M^2 and therefore M has at least 25 hexagons.

Case 2. Each of B_M^i $(i = 1,2)$ has less than 10 hexagons. By Lemmas 9, 6 and 7, each of B_M^i and B_H^i $(i = 1,2)$ is a crown or a crown-plus or the double-crown-minus. There are several subcases:

Subcase 1. The ear of B_M^i is 3-type in B_M^i $(i = 1,2)$. By Lemma 9, they have no 4- and 5-type hexagons in themselves. By Lemma 6, B_M^1 and B_M^2 are crowns and each has 6 removable 3-type hexagons in itself. Except the ears, all other 3-type hexagons of B_M^1 and B_M^2 are also 3-type in M. Thus B_M^1 and B_M^2 contain at least 10 3-type hexagons of M. These 3-type hexagons are mapped under f^- onto 10 non-removable 3-type hexagons of H. None of them is contained in B_H^1 or B_H^2 (otherwise one of the ears of B_H^1 and B_H^2, say the ear of B_H^1, will be 3-type in H and thus 5-type in B_H^1. This contradicts Lemma 9. If $h(H) = 24$, then B_H^1 and B_H^2 together have 14 hexagons and therefore are crowns, and H is the union of B_H^i and $f^-(S_M^i)$ $(i = 1,2)$. Since each of S_M^i $(i = 1,2)$ contributes a segment 33333 to the BE code of M, $f^-(S_M^i)$ contributes a segment 33333 to the BE code of H $(i = 1,2)$ too. In order to maintain this property and the fact that B_H^i is a crown $(i = 1,2)$, $f^-(S_M^i)$ and B_H^i $(i = 1,2)$ have to be connected in a unique way as shown in Fig. 4. By the symmetrical position of H and M in the above reasoning, M is also equal to the fusene as shown in Fig. 4.

Subcase 2. The ear of B_M^i is 4-type in B_M^i $(i = 1,2)$. By Lemmas 9, 6 and 7, B_M^i $(i = 1,2)$ is either a crown-plus or a double-crown-minus.

(i) If both B_M^1 and B_M^2 are crown-pluses, then S_M^i contributes a segment 233332 to the BE code of M $(i=1,2)$. Thus $f^-(S_M^i)$ contributes a segment 233332 to the BE code of H $(i=1,2)$. Note that each hexagon in $f^-(S_M^i)$ is non-removable in H and these 3-type hexagons in $f^-(S_M^1)$ are completely different from those in $f^-(S_M^2)$. Thus $f^-(S_M^1)$ and $f^-(S_M^2)$ have at most one hexagon in common (otherwise, H will not be simply connected). So there are at least 11 non-removable hexagons in H and each is 2- or 3-type. If the ear of B_H^i is 4-type, then it has at least 7 hexagons (6 removable hexagons plus at least one more interior hexagon) which are different from the 11 non-removable hexagons. If the ear of B_H^i is 3-type, then it is 1-type in H. Thus B_H^i has at least 7 hexagons which are different from the 11 hexagons mentioned above. In any of the above two cases, H has at least 25 hexagons.

(ii) Both B_M^1 and B_M^2 are the double-crown-minus. Then B_M^1 and B_M^2 have 18 hexagons. By Lemmas 6 and 7, B_H^1 and B_H^2 have at least 8 hexagons which are 3-type and removable in H. Thus under f, these hexagons are mapped onto 3-type non-removable hexagons of M. So M has at least 8 non-removable 3-type hexagons which do not belong to B_M^1 and B_M^2. Thus M has at least 26 hexagons.

(iii) One of B_M^1 and B_M^2 is the double-crown-minus and the other is the crown-plus. So both have in total at least 17 hexagons. By Lemmas 6 and 7, B_H^1 and B_H^2 have at least 8 hexagons which are 3-type and removable in H. Thus under f, these hexagons are mapped onto 3-type non-removable hexagons of M. So M has at least 8 non-removable 3-type hexagons. Since the ear of B_M^i $(i=1,2)$ is either 1- or 2-type in M, the hexagons in B_M^i $(i=1,2)$ are different from these 8 non-removable 3-type hexagons. Thus M has at least 25 hexagons.

Subcase 3. One of the ears of B_M^i $(i=1,2)$ is 3-type and the other is 4-type. If both ears of B_H^i $(i=1,2)$ are 3-type in themselves, by symmetry, this is Subcase 1. If both of the ears of B_H^i $(i=1,2)$ are 4-type in themselves, this is Subcase 2. The remaining case is one of the ears of B_H^i $(i=1,2)$ is 3-type and the other is 4-type. Without loss of generality, let the ears of B_M^1 and B_H^1 be 3-type in themselves, respectively. Hence B_M^1 and B_H^1 are crowns and B_M^2 (B_H^2) is either a crown-plus or a double-crown-minus. B_M^1 has 5 3-type removable hexagons in M which contribute a segment 33 333 to the BE code of M. If B_M^2 has 8 hexagons, it is a crown-plus. So the removable hexagons of M in B_M^2 contribute a segment 233332 to the BE code of M. Note that these removable hexagons both in B_M^1 and B_M^2 mentioned above are mapped under f^- onto non-removable hexagons of H with the same type. There are at least 11 such non-removable hexagons in H. None of B_H^1's hexagons (which are either 3-type or 1-type hexagons in H) is among these 11 hexagons. Since B_H^2 has at least 8 hexagons and its ear may be a 2-type hexagon in H, it contributes at least 7 hexagons which are different from these 11 non-removable hexagons. Thus H has at least 25 hexagons. If B_M^2 has 9 hexagons, then B_M^2 is a double-crown-minus. The removable hexagons of M in B_M^2 contributes a segment 13 33323 to the BE code of M. Thus both B_M^1 and B_M^2 contains at least 10 removable 3-type hexagons of M which are mapped under f^- to non-removable 3-type hexagons of H. Hence, both B_H^1 and

B_H^2 have at least 15 hexagons and none of them is among the 10 non-removable 3-type hexagons mentioned above. Thus H has at least 25 hexagon. □

Theorem 3. *Let (H_1, H_2) be an SBE pair with H_1 and H_2 not isomorphic, then they have at least 25 hexagons. Moreover, such a pair exists with 25 hexagons.*

Proof. Let f^0 be a boundary symmetry mapping from H_1 to H_2. If under f each removable hexagon of H_1 is mapped onto a non-removable hexagon of H_2, then (H_1, H_2) is an irreducible pair. By Lemma 10, H_1 as well as H_2 has at least 24 hexagons. If H_1 has 24 hexagons, then H_1 is isomorphic to H_2 by Lemma 10. This is a contradiction. Thus $h(H_1) = h(H_2) \geqslant 25$. Now let s_1 be a removable hexagon of H_1 such that $f^0(s_1)$ is removable in H_2. Let H_1^1 be the subgraph consisting of all the hexagons of H_1 except s_1 and H_2^1 the subgraph consisting of all the hexagons of H_2 except $f^0(s_1)$. Then $(H_1 - s_1, H_2^1 - f^0(s_1))$ is an SBE pair. Let f^1 be the boundary symmetry mapping from $V(H_1 - s_1)$ to $V(H_2 - f^0(s_1))$ such that $f^0(v) = f^1(v)$ for each v in $B(H_1) \cap B(H_1 - s_1)$. If under f^1 each removable hexagon is mapped onto a non-removable hexagon, then $(H_1 - s_1, H_2 - f^0(s_1))$ is an irreducible SBE pair. By Lemma 10, $h(H_1 - s_1) \geqslant 24$ and thus $h(H_1) \geqslant 25$. Otherwise, there is a removable hexagon s_2 of $H_1 - s_1$ mapped onto a removable hexagon $f^1(s_2)$ of $H_2 - f^0(s_1)$. Then $(H_1 - s_1 - s_2, H_2 - f^0(s_1) - f^1(s_2))$ is an SBE pair. Let f^2 be the boundary symmetry mapping from $H_1 - s_1 - s_2$ to $H_2 - f^0(s_1) - f^1(s_2)$ such that $f^2(v) = f^1(v)$ for each v in $B(H_1 - s_1) \cap B(H_1 - s_1 - s_2)$. If each removable hexagon is mapped onto a non-removable hexagon under f^2, then $(H_1 - s_1 - s_2, H_2 - f^0(s_1) - f^1(s_2))$ is irreducible. By Lemma 10, $h(H_1 - s_1 - s_2) \geqslant 24$. Thus the theorem is true. Otherwise, we can iterate the previous step as above until either the remaining pair is irreducible or each of the remaining fusenes has one hexagon. Assume that after i steps, the process stops. Then there is an SBE pair $(H_1 - s_1 - s_2 - \cdots - s_i, H_2 - f^0(s_1) - f^1(s_2) - \cdots - f^{i-1}(s_i))$ and with the boundary symmetry mapping f^i. If $H_1 - s_1 - s_2 - \cdots - s_i$ has only one hexagon, then $H_1 - s_1 - s_2 - \cdots - s_i$ is isomorphic to $H_2 - f^0(s_1) - f^1(s_2) - \cdots - f^{i-1}(s_i)$. Define $F = f^0 + f^1 + \cdots + f^i$, a one-to-one mapping from $V(H_1)$ to $V(H_2)$, such that $F(v) = f^j(v)$ for a vertex v in $V(H_1) \cap V(H_1 - s_1 - s_2 - \cdots - s_j)$. By the choice of f^j $(j = 0, \ldots, i)$, one can check that F is an isomorphism from H_1 to H_2. This is a contradiction. Thus $(H_1 - s_1 - s_2 - \cdots - s_i, H_2 - f^0(s_1) - f^1(s_2) - \cdots - f^{i-1}(s_i))$ is an irreducible SBE pair. By the same reasoning as before, $h(H_1 - s_1 - s_2 - \cdots - s_i) \geqslant 24$. Therefore $h(H_1) \geqslant 25$.

Fig. 2 gives an SBE pair of non-isomorphic helicenes with 25 hexagons. The theorem is proved. □

Corollary 4. *Any fusene with at most 24 hexagons is uniquely determined by its boundary edge code.*

In general, fusenes are not uniquely determined by their boundaries, but for geometrically planar fusenes, the following is true:

Theorem 4. *Let H and M be two geometrically planar fusenes with the same BE code. Then H and M are isomorphic.*

Proof. Without loss of generality, let H and M have more than one hexagon. Embed H and M into the infinite hexagonal lattice so that $B(H)$ coincides with $B(M)$. Then for each v in $V(H)$, there is a unique vertex v' in $V(M)$ which occupies the same position as v. This naturally derives a one-to-one mapping from $V(H)$ to $V(M)$ which maps only adjacent vertices to adjacent vertices. It is an isomorphism from H to M. □

4. Open problems

Checking the irreducible pair (H,M) with 24 hexagons in Lemma 10, we make the following observation: there are some fusenes whose symmetry group is smaller than its boundary symmetry group (the symmetry group and the boundary symmetry group of a helicene contain all the symmetry mappings and the boundary symmetry mapping, respectively). We can partition all fusenes into two groups:

Group A contains all the fusenes whose symmetry group is the same as its boundary symmetry group. Fusenes in Group A are said to be type-A fusenes.

Group B contains fusenes not in Group A. Fusenes in Group B are said to be type-B fusenes.

Problem 1. Characterize the fusenes in Group B.

The two helicenes in Fig. 2 forms a reducible pair. There are some irreducible SBE pairs in which the two helicenes are not isomorphic. But their number of hexagons is larger than 25.

Problem 2. Is there an irreducible SBE pair (H,M) such that $h(H)=h(M)=25$ and H and M are not isomorphic?

Acknowledgements

Work of the first author was supported in part by the National Natural Science Foundation of PRC. Work of the second author was supported by grants NSERC Grant GP0105574, and FCAR Grant 92-EQ-1048 and a Grant from CETAI-HEC. The authors thank for Prof. Gunnar Brinkmann (Fakultät fur Mathematik, Bielefeld University, Germany) for helpful discussions and suggestions.

References

[1] D. Avis, K. Fukuda, Reverse search for enumeration, Discrete Appl. Math. 65 (1996) 21–46.

[2] A.T. Balaban, F. Harary, Enumeration and proposed nomenclature of benzenoid cata-condensed polycyclic aromatic hydrocarbons, Tetrahedron 24 (1967) 2505–2516.
[3] K. Balasubramanian, Recent chemical applications of computational combinatorics and graph theory, in: D.H. Rouvray (Ed.), Computational Chemical Graph Theory, Nova Science, New York, 1990.
[4] D. Bonchev, D.H. Rouvray, Chemical Graph Theory, Introduction and Fundamentals, Abacus Press, Gordon and Breach, New York, 1991.
[5] D. Bonchev, D.H. Rouvray, Chemical Graph Theory, Reactivity and Kinetics, Abacus Press, Gordon and Breach, New York, 1992.
[6] J. Brunvoll, B.N. Cyvin, S.J. Cyvin, Enumeration of benzenoid systems and other polyhexes, Topics Curr. Chem. 162 (1992) 65–180.
[7] G. Caporossi, P. Hansen, Enumeration of polyhex hydrocarbons to $h = 21$, J. Chem. Inform. Comput. Sci. 38 (1998) 610–619.
[8] G. Caporossi, P. Hansen, M. Zheng, Enumeration of fusenes to $h = 20$. in: P. Hansen, P. Fowler, M. Zheng (Eds.), Discrete Mathematical Chemistry, DIMACS Series on Discrete Mathematics and Theoretical Computer Science, AMS, Providence, RI 51 (2000) 63–78.
[9] I.A. Faradzev, Constructive enumeration of combinatorial objects, in: Problèmes combinatoires et théorie des graphes, eds. J.C. Bermond, et al., Colloque Intern., CNRS Vol. 260 CNRS, Paris, 1978, pp. 131–135.
[10] I. Gutman, S.J. Cyvin, Introduction to the Theory of Benzenoid Hydrocarbons, Springer, Berlin, 1989.
[11] P. Hansen, C. Lebatteux, M. Zheng, The boundary-edges code for polyhexes, Theochem. J. Mol. Struct. 363 (1996) 237–247.
[12] W. Herndon, A.J. Bruce, Perimeter code for benzenoid aromatic hydrocarbons, Stud. Phys. Theoret. Chem. 51 (1987) 491–513.
[13] H. Hosoya, Some recent advances in counting polynomials in chemical graph theory, in: H.H. Rouvray (Ed.), Computational Chemical Graph Theory, Nova Science, New York, 1990.
[14] J.V. Knop, W.R. Müller, K. Szymanski, Computer-oriented molecular codes, in: H.H. Rouvray (Ed.), Computational Chemical Graph Theory, Nova Science, New York, 1990.
[15] J.V. Knop, W.R. Müller, K. Szymanski, N. Trinajstić, Use of small computers for large computations: enumeration of polyhex hydrocarbons, J. Chem. Inform. Comput. Sci. 30 (1990) 159–160.
[16] B.D. McKay, Isomorph-free exhaustive generation, J. Algorithms 26 (1998) 306–324.
[17] W.R. Müller, K. Szymanski, J.V. Knop, S. Nikolić, N. Trinajstić, On the enumeration and generation of polyhex hydrocarbons, J. Comput. Chem. 11 (1990) 223–235.
[18] W.R. Müller, K. Szymanski, N. Trinajstić, On counting polyhex hydrocarbons, Croat. Chem. Acta 62 (1989) 481–483.
[19] R.C. Read, Everyone a winner, Ann. Discrete Math. 2 (1978) 107–120.
[20] D.H. Rouvray, Computational Chemical Graph Theory, Nova Science, New York, 1990.
[21] R. Tošić, D. Mašulović, I. Stojmenović, J. Brunvoll, S.J. Cyvin, B.J. Cyvin, Enumeration of polyhex hydrocarbons to $h = 17$, J. Chem. Inform. Comput. Sci. 35 (1995) 181–187.
[22] N. Trinajstić, Chemical Graph Theory, CRC Press, Boca Raton FL, 1992.