match no. 19 pp. 219-228 1986

TOPOLOGICAL PROPERTIES OF BENZENOID SYSTEMS. XXXVIII. THE BOUNDARY CODE

Ratko Tošić*, Rade Doroslovački** and Ivan Gutman***

* Institute of Mathematics, Faculty of Science, University of Novi Sad, 21000 Novi Sad, Dr.Ilije Djuričića 4, Yugoslavia

** Institute for Applied Basic Disciplines, Faculty of Engineering, University of Novi Sad, 21000 Novi Sad, Veljka Vlahovića 3, Yugoslavia, and

*** Faculty of Science, University of Kragujevac, P.O.Box 60, 34000 Kragujevac, Yugoslavia

(Received: May 1985)

ABSTRACT. The boundary code is a word on a six-letter alphabet which uniquely determines the perimeter of a benzenoid system and therefore determines the benzenoid system itself. Necessary and sufficient conditions are given for a word on a six-letter alphabet to be the boundary code of a benzenoid system. Benzenoid systems having perimeters of length 28 or less are enumerated.

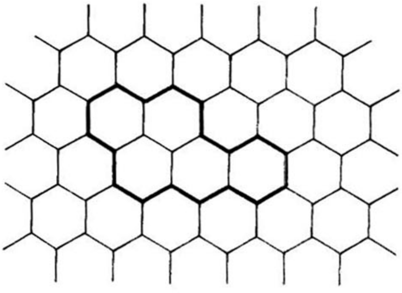
1. Introduction

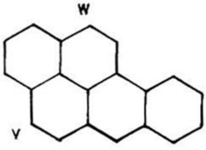
Hundreds of papers dealing with topological properties of benzenoid hydrocarbons have been published in the last few decades[1-3]. In the great majority of these investigations the notion of a benzenoid system[4] (or, when graph-theoretical formalism is used, of a benzenoid graph) is understood as intuitively evident and no efforts are made to provide a rigorous mathematical definition.

Usually one describes benzenoid systems as figures obtained by arranging congruent regular hexagons in a plane, so that two hexagons are either disjoint or have exactly one common edge. Such figures are required to be simply connected. The network formed by a benzenoid system is then interpreted as a benzenoid graph.

Another approach is to consider a hexagonal lattice embedded in a plane. A cycle of this lattice represents the boundary (or as one traditionally says: the perimeter) of a benzenoid system. It is evident that the perimeter uniquely determines the corresponding benzenoid system[1].

As an example we present a cycle on the hexagonal lattice, being the perimeter of the benzenoid system B.





B

Knop et al.[3] and independently two of the present authors[5,6] proposed to characterize a benzenoid system by associating to its perimeter a sequence of symbols from a six-letter alphabet. The name boundary code was given to this sequence in[3] and we shall use it throughout the present paper.

Before defining the boundary code we would like to remind the reader to some notions from combinatorics.

The set of the first k natural numbers is denoted by $\mathbb{N}_k$. Hence $\mathbb{N}_k = \{1,2,\ldots,k\}$. The set $\mathbb{A} = \{a_1,a_2,\ldots,a_k\}$ is called the alphabet if for all $i \in \mathbb{N}_k$, a_i are arbitrary symbols. The elements of $\mathbb{A}$ are then the letters of the alphabet and $\mathbb{A}$ is a k-letter alphabet.

If $x \in \mathbb{A}^n$ i.e. if $x = (a_1,a_2,\ldots,a_n)$ is an ordered n-tuple with components from $\mathbb{A}$, we say that x is a word of the length n on the alphabet $\mathbb{A}$. For the sake of brevity we shall write x as $a_1a_2\ldots a_n$.

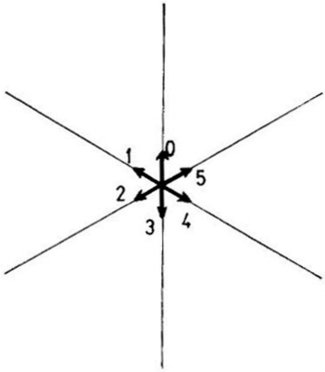
A subword of the length k of the word $a_1a_2\ldots a_n$ is any word $a_sa_{s+1}\ldots a_{s+k-1}$ where $s \in \mathbb{N}_{n-k+1}$ and $k \in \mathbb{N}_n$.

The set of all words of finite length on the alphabet $\mathbb{A}$ will be denoted by $\mathbb{A}^*$.

The number of ways in which a subword y occurs in a word $x \in \mathbb{A}^*$ is denoted by $k_y(x)$. In particular, the number of ways in which the letter $a \in \mathbb{A}$ occurs in the word $x \in \mathbb{A}^*$ is $k_a(x)$.

2. Characterization of the Perimeter by Words on the Alphabet {0,1,2,3,4,5}

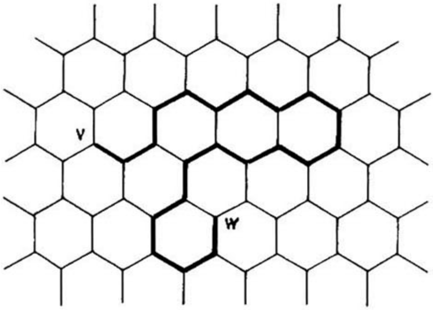
Through every point of the hexagonal lattice one can set three straight lines, such that every edge of the lattice is parallel to exactly one of these lines. Consider such three lines and direct them. The unit vectors of these lines are denoted by 0, 1 and 2 so that the angle between 0 and 1 is equal to $\pi/3$ whereas the angle between 0 and 2 is $2\pi/3$. The oppositely directed unit vectors will be denoted by 3,4 and 5, respectively.



The set $A = \{0,1,2,3,4,5\}$ will be our alphabet[7].

It is evident that every directed edge of the hexagonal lattice is in a one-to-one correspondence with an element of A. Hence we have defined a function which maps the set of all finite directed paths of the hexagonal lattice into A^*.

For example, we present a path on the hexagonal lattice connecting the vertices v and w.



This path can be directed in two ways. It either starts at the vertex v and ends at the vertex w or vice versa. If this path is directed from the vertex v to the vertex w, then it corresponds to the word 450545454321212323450. If the same path is directed oppositely, namely from w to v, then it corresponds to the word 3210505454501212123 21.

The words which correspond to the two opposite orientations of a given path of the hexagonal lattice are related in the following way. Let $x = a_1a_2\ldots a_{n-1}a_n$ and $y = b_1b_2\ldots b_{n-1}b_n$ be two such words. Then

$$a_1 - b_n \equiv a_2 - b_{n-1} \equiv \ldots \equiv a_{n-1} - b_2 \equiv a_n - b_1 \equiv 3 \pmod 6 .$$

This means that by considering the letters of x as ordinary integers and by adding 3 modulo 6 to them we arrive at a word which is equal to the word obtained by reading the letters of y from right to left.

This property of the path codes can be easily verified on the above example:

$$450545454321212323450 \ + \ 333333333333333333333 \ =$$

$$783878787654545656783 \ \equiv \ 123212121054545050123 \pmod{6} \quad .$$

A cycle of length n of the hexagonal lattice determines 2n distinct closed directed paths, since one can start from any of the n vertices of the cycle and direct the path in two different ways. Hence a cycle of length n can be represented by 2n distinct words from A^n. These 2n words correspond, of course, to the same benzenoid systems and are called[3] its boundary codes.

For example, the following four words from A^{18} are the boundary codes of the benzenoid system B. (The graph of B is given in the previous section.)

$$x_1 = 010545434543212121$$

$$x_2 = 454545012101212343$$

$$x_3 = 434543212121010545$$

$$x_4 = 212343454545012101$$

If we start from the vertex v, we obtain x_1 and x_2 ; if the starting vertex is w then x_3 and x_4 are obtained. Additional fourteen boundary codes for the same boundary would be obtained by choosing the starting vertex different from v or w.

The problem how to decide whether two words from $\mathcal{A}^*$ represent the boundary code of the same benzenoid system was discussed in detail in[3,5,6]. In the present work we shall be interested in a related question, namely how to recognize which words from $\mathcal{A}^*$ are boundary codes.

3. Characterization of the Boundary Code

The following statement gives the necessary and sufficient conditions for a word from $\mathcal{A}^*$ to be a boundary code of a benzenoid system.

Theorem 1. The word $x = a_1 a_2 \ldots a_n \in \mathcal{A}^n$ is a map of a closed directed path of the hexagonal lattice if and only if the conditions (a),(b) and (c) are simultaneously satisfied.

(a) For all $i \in \mathbb{N}_{n-1}$, $a_{i+1} \equiv a_i + 1 \pmod 6$ or $a_{i+1} \equiv a_i - 1 \pmod 6$.

(b) $k_0(x) = k_3(x)$ and $k_1(x) = k_4(x)$ and $k_2(x) = k_5(x)$.

(c) For every subword y of x, $y \neq x$, at least one of the equalities in (b) is not obeyed, i.e. either $k_0(y) \neq k_3(y)$ or $k_1(y) \neq k_4(y)$ or $k_2(y) \neq k_5(y)$.

The "if" part of Theorem 1 is elementary. Condition (a) simply expresses the fact that the closed path is continuous. Condition (b) guarantees that the path is closed whereas the condition (c) forbids the closure of the cycle with less than n edges.

That the conditions (a)-(c) are also sufficient is less easy to see. The proof is somewhat lengthy and can be found in[5,6].

Theorem 1 enables one to generate all non-isomorphic benzenoid systems by generating the words of A^* which fulfill the conditions (a),(b) and (c). This latter task seems to be much easier. A FORTRAN program has been written for the enumeration of benzenoid systems with a given perimeter length. The results obtained are presented in the following table. H(n) denotes the number of non-isomorphic benzenoid systems having a perimeter of the length n.

n	6	8	10	12	14	16	18	20	22	24	26	28
H(n)	1	0	1	1	3	2	12	14	50	97	312	744

ACKNOWLEDGMENT

One of the authors (I.G.) thanks the Alexander von Humboldt Foundation for financial support and the staff of the Max-Planck-Institut für Strahlenchemie in Mülheim for assistance and hospitality.

References

1. For review on the topological properties of benzenoid molecules see: I.Gutman, Bull.Soc.Chim.Beograd 47, 453 (1982).
2. The following papers on benzenoid molecules, published in the last ten years in just one journal should illustrate the intensity of the research in this area:
   A.T.Balaban, Match 2,51 (1976); O.E.Polansky and D.H.Rouvray, Ibid. 2,63 (1976); 2,91 (1976); 3, 97 (1977); O.E. Polansky and I.Gutman, Ibid. 4, 219 (1978); 8, 269 (1980); S.B.Elk, Ibid. 8, 121 (1980); 13, 239 (1982); 17, 255 (1985); S.El-Basil, Ibid. 11, 97 (1981); 13, 183 (1982); 13, 199 (1982); 13, 209 (1982); I.Gutman, Ibid. 11, 127 (1981); 13, 173 (1982); 14, 139 (1983); 17, 3 (1985); O.E. Polansky and N.N.Tyutyulkov, Ibid. 12, 177 (1981); S.J. Cyvin, Ibid. 13, 167 (1982); O.E.Polansky, Ibid. 14, 71 (1983); J.R.Dias, Ibid. 14, 83 (1983); A.T.Balaban and I. Tomescu, Ibid. 14, 155 (1983); 17, 91 (1985); M.Zander, Ibid. 14, 183 (1983); S.El-Basil and A.S.Shalabi, Ibid. 14, 191 (1983); 17, 11 (1985); I.Gutman, O.E.Polansky and M.Zander, Ibid. 15, 145 (1984); R.S.Lall, Ibid. 15, 251 (1984); J.V.Knop, K.Szymanski and N.Trinajstić, Ibid. 16, 103 (1984); J.V.Knop, K.Szymanski, Z.Jeričević and N.Trinajstić, Ibid. 16, 119 (1984);S.El-Basil, S.Botros and M. Ismail, Ibid. 17, 45 (1985); I.Gutman, S.Obenland and W. Schmidt, Ibid. 17, 75 (1985).

3. J.V.Knop, K.Szymanski, Z.Jeričević and N.Trinajstić, J.Comput.Chem. 4, 23 (1983); J.V.Knop, K.Szymanski, G. Jashari and N.Trinajstić, Croat.Chem.Acta 56, 443 (1983); N.Trinajstić, J.V.Knop, W.R.Müller and K.Szymanski, Pure Appl.Chem. 55, 379 (1983).
4. In addition to "benzenoid system" the names "polyhexes", "fusene" and "PAH6" are used in the chemical literature. Mathematicians call the same objects "hexagonal systems", "hexagonal animals" or "hexaominoes".
5. R.Doroslovački, M.Sc.Thesis, University of Novi Sad, 1984.
6. R.Doroslovački and R.Tošić, Review of Research Fac.Sci. Univ.Novi Sad, Ser.Math. 14a, to be published.
7. Note that in the papers by Knop et al.[3] the alphabet {1,2,3,4,5,6} has been used. The advantage of our choice is evident from the condition (a) of Theorem 1.