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Computer Search for Isospectral Benzenoid Graphs*

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Abstract

In this note, we propose a new procedure for the computer search of isospectral benzenoid graphs (IBGs). For benzenoid graphs with less then 14 hexagons, we find three pairs of IBGs with 12 hexagons and odd number of vertices. In addition, we find no iso-laplacian-spectral benzenoid graphs with less than 14 hexagons.

1 Introduction

Graph isospectrality is continuously drawing the attention of researchers in the fields of graph theory and mathematical chemistry. In [4], the problem of existence of isospectral benzenoid graphs (IBGs) was first mentioned. In [5], it was shown that there are no IBGs with 8 and fewer hexagons. In [1,2], Babić and Gutman proposed a Heilbronner-like procedure for constructing IBGs with an odd number of vertices. In [8], Zheng et al. found also the IBGs with 9 hexagons by computing the characteristic polynomial. In [3], Caporossi and Hansen proposed an algorithm based on the boundary edges code (BEC)

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of benzenoid graphs, which led to the enumeration of polyhexes with 21 hexagons. For a precise definition of BEC see [3].

A benzenoid graph is defined [6] as a graph induced by the vertices lying on and inside the cycle in the hexagonal lattice. The spectrum of the graph G denotes the set of eigenvalues of the corresponding adjacency matrix $A(G)$. Non-isomorphic graphs having equal spectra are called isospectral. Related definitions and terms refer to [1].

Let $D(G)$ be the diagonal matrix indexed by vertices set $V(G)$ and with vertex degrees on the diagonal. The difference $L(G) = D(G) - A(G)$ is called the Laplace matrix of G. Non-isomorphic graphs having equal Laplacian-spectra are called iso-laplacian-spectral.

In this note, we propose two procedures to build adjacency matrices of benzenoid graphs by BECs, and search IBGs by computing characteristic polynomials of those matrices.

2 Procedure

It is well known that isospectral graphs have same characteristic polynomials with integer coefficients. To compute the characteristic polynomial of a benzenoid graph, we design the following procedure.

Procedure 1. Build the adjacency matrix of a benzenoid graph by its BEC.

Input: The BEC of a benzenoid graph G.

Output: $A(G)$

begin

1. Start from the origin of cartesian coordinate system, compute coordinates of external vertices of G by its BEC, save them in a matrix W and build the corresponding adjacency matrix A.

2. Compute coordinates of internal neighbor vertices of all external vertices with degree three. If a pair of coordinates already is in W, then modify A only; else, add the coordinates to W and modify A.

3. For those newly added internal vertices, compute coordinates of their neighbor vertices. If a pair of coordinates already is in W, then modify A only; else, add the coordinates to W and modify A.

4. Repeat step 3 until there is no newly added vertex.

end

With increasing of the number of hexagons, the size of adjacency matrix of the corresponding benzenoid graph will grow rapidly. In order to simplify the comparison, we adopt the following procedure.

Procedure 2. Search of IBGs.

Input: BECs of all benzenoid graphs with n hexagons.

Output: BECs of IBGs and coefficients of their characteristic polynomials.

begin

1. Compute the adjacency matrix of every benzenoid graph with n hexagons by Procedure 1, sum absolute values of coefficients of every characteristic polynomial and save the results.

2. Sort the results of Step 1 and search out those benzenoid graphs with equal sum value.

3. From the results of Step 2, search out IBGs with n hexagons and output coefficients of their characteristic polynomials.

end

3 Results

Using the above procedures, we searched all benzenoid graphs with less then 14 hexagons. Besides the IBGs with 9 hexagons, we found only the following three pairs of IBGs with 12 hexagons and odd number of vertices, which are concordant with the results in [1,2].

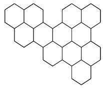
(a) (b)

Fig. 1: (a)BEC:441214412144121, (b)BEC:431134311343113

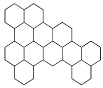
(a) (b)

Fig. 2: (a)BEC:441331314413121, (b)BEC:431413134313113

i) coefficients of characteristic polynomial of IBGs in Fig.1: 1, 0, -54, 0, 1344, 0, -20492, 0, 214593, 0, -1640202, 0, 9492213, 0, -42586062, 0, 150422358, 0, -422469922, 0,



(a)



(b)

Fig. 3: (a)BEC:4314311343131, (b)BEC:4413134134121

948813519, 0, -1707670494, 0, 2460307814, 0, -2824938336, 0, 2563801587, 0, -1815451002, 0, 983802753, 0, -396471996, 0, 113771385, 0, -21681918, 0, 2421009, 0, -118098, 0.

ii) coefficients of characteristic polynomial of IBGs in Fig.2: 1, 0, -54, 0, 1344, 0, -20492, 0, 214595, 0, -1640278, 0, 9493545, 0, -42600310, 0, 150526182, 0, -423015200, 0, 950945129, 0, -1713990994, 0, 2474667295, 0, -2850018426, 0, 2597380734, 0, -1849577584, 0, 1009635570, 0, -410566240, 0, 119003580, 0, -22863780, 0, 2543481, 0, -118098, 0.

iii) coefficients of characteristic polynomial of IBGs in Fig.3: 1, 0, -52, 0, 1241, 0, -18061, 0, 179651, 0, -1297380, 0, 7053295, 0, -29539945, 0, 96727787, 0, -249897209, 0, 511758294, 0, -831448058, 0, 1068701006, 0, -1079447531, 0, 847028926, 0, -507313500, 0, 225820619, 0, -71704632, 0, 15188456, 0, -1896336, 0, 103428, 0.

In addition, using the above method, we find no iso-laplacian-spectral benzenoid graphs with less then 14 hexagons.

References

[1] D. Babić, I. Gutman, On isospectral benzenoid graphs, *J. Math. Chem.* **9** (1992) 261–278.

[2] D. Babić, Isospectral benzenoid graphs with an odd number of vertices, *J. Math. Chem.* **12** (1993) 137–146.

[3] G. Caporossi, P. Hansen, Enumeration of polyhex hydrocarbons to $h = 21$, *J. Chem. Inf. Comput. Sci* **38** (1998) 610–619.

[4] J. Cioslowski, A conjecture on benzenoid graphs, *J. Math. Chem.* **6** (1991) 111–111.

[5] I. Gutman, S. Marković, V. Grbović, The smallest pair of isospectral benzenoid systems, *J. Serb. Chem. Soc.* **56** (1991) 553–554.

[6] I. Gutman, S.J. Cyvin, *Introduction to the Theory of Benzenoid Hydrocarbons*, Springer–Verlag, Berlin, 1989.

[7] J. Knop, W. Müller, K. Szymanski, N. Trinajstić, Use of small computers for large computations: Enumeration of polyhex hydro-carbons, *J. Chem. Inf. Comput. Sci* **30** (1990) 159–160.

[8] S. Zheng, Z. Wang, J. Zhang, X. Xin, A result of searching for isospectral benzenoid graphs, *J. Xinjiang Unive. (Nat. Sci. Ser.)* **13** (1996) 21,28.