*Research Paper*

The adjacency matrix of some hexagonal systems

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Abstract. It is well known that in the graph theory the adjacency matrix is an important invariant [5]. Especially, the adjacency matrix is also very important in the theory of chemical graphs, for example, in obtaining graph energy. In this paper, the general form of the adjacency matrices of some hexagonal systems will be determined.

Keywords: Adjacency matrix, $Pr(2, n)$, $M(3, n)$, $Ch(2, 2, n)$, $S(n)$, $Z(4, n)$

Mathematics Subject Classification (2010): 05C50.

1 Introduction

Suppose M is a molecule and X is the set of all atoms of M . Two members of X are assumed to be adjacent, if there is a chemical bond between them. This gives us a simple graph which is called the **chemical graph** of M . This simple graph is the main object of chemical graph theory. A hexagonal system (benzenoid graph) H , is a finite connected plane graph without cut vertices in which every interior region is bounded by a regular hexagon. It is well known that benzenoid graphs possess very natural chemical background. In particular, the skeleton of carbon atoms in a benzenoid hydrocarbon is a benzenoid graph, [4]. For systems with a large number of atoms and with a dense network of bonds, determining the topological invariants of chemical structures in many cases provides a basis for understanding difficult theoretical problems. With the knowledge of topological descriptors, a better qualitative understanding of different molecular aspects in their chemistry and physics can be obtained [3]. An $n \times n$ matrix $A = [a_{i,j}]$ is called symmetric if $a_{ij} = a_{ji}$ and centrosymmetric when its entries

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satisfy $a_{ij} = a_{n-i+1, n-j+1}$ for $1 \leq i, j \leq n$.

Let X be an n -vertex simple graph containing n vertices u_1, u_2, \dots, u_n . The adjacency matrix $A(X) = [t_{ij}]$ is a matrix for which $t_{ii} = 0, 1 \leq i \leq n$, and $t_{ij} = 1, i \neq j$, if and only if u_i and u_j are adjacent. We use the famous book of Biggs [5] for important properties of this matrix.

Determining the adjacency matrix in graph theory is always important. If this matrix is available, the graphical parameters of a graph can be calculated, including the characteristic polynomial, Wiener index, eigenvectors, etc. The authors have presented an algorithm similar to this method to obtain the adjacency matrix of a set of hexagonal systems. See [6] for more details. Our other notations are standard and our chemical graphs are drawn with the aid of ChemDraw [2]. In this article, Chemdraw software is used to draw graphs [2], and matrices are written under the pattern presented in this article using Mathematica software, [7]. Now by having the adjacency matrix and reusing the mathematica software, it is possible to obtain invariants such as determinant, permanent, energy, etc.

The purpose of this article is to provide a general method for determining the adjacency matrix of some hexagonal systems, where the adjacency matrix of six of them is given here.

2 Adjacency matrices of $Pr(2, n)$

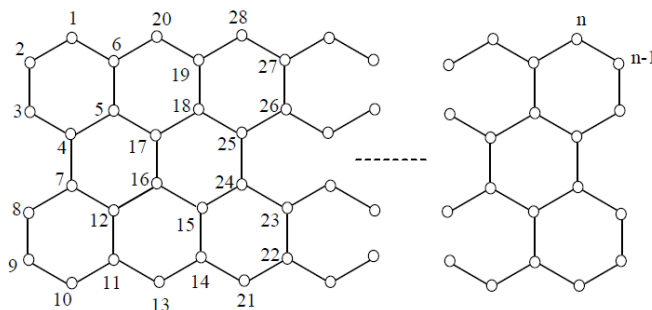


Figure 1. $Pr(2, n); n = 20 + 8(k - 1); k = 1, 2, \dots$

In [1] a set of regular 3- and 4-tier benzenoid strips was presented. The aim of this section is to calculate the adjacency matrices of these benzenoid strips in general. Suppose that $A_{n \times n} = [a_{i,j}], 1 \leq i, j \leq n$, is the adjacency matrix of $pr(2, n)$. To calculate the adjacency matrix of $pr(2, n)$, we have to determine all entries which are equal to one. To determine the adjacency matrix, we will do as follows: consider the values t as $t = \lfloor \frac{n}{8} \rfloor - 2$ and $m = \lfloor \frac{n}{8} \rfloor - 1$, where $\lfloor x \rfloor$ denotes the integer part of x and gives the largest integer less than or equal to x . We have shown the labeling in Figure 1 that the $(i, i + 1); 1 \leq i \leq n - 1, i \neq 12 + 8(k - 1); 1 \leq k \leq m$ pairs of their value in the adjacency matrix is equal to 1.

Pairs $(18, 25), (26, 33), \dots$ whose components are arithmetic sequences with the first

3 Adjacency matrices of $M(3, n)$

In this section we present the adjacency matrices of the class $M(3, n)$ in general.

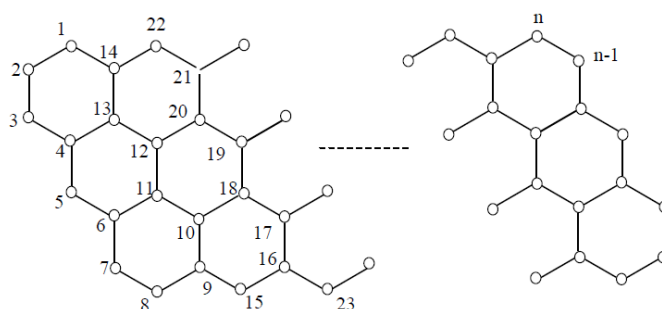


Figure 2. Parallelograms $M(3, n), n = 22 + 8(k - 1); k = 1, 2, \dots$

Let $B_{n \times n} = [a_{i,j}], 1 \leq i, j \leq n$, be the adjacency matrix of $M(3, n)$. We first present a labeling of the graph which is important in our calculations.

To calculate the adjacency matrix of $M(3, n)$, we have to determine all entries which are equal to one. Define $t = \lfloor \frac{n}{8} \rfloor - 2$ and $m = \lfloor \frac{n}{8} \rfloor - 1$. If $1 \leq k \leq t$ then all entries corresponding to the following four sets of ordered pairs are equal:

$$\begin{aligned} & (19 + 8(k + 1), 28 + 8(k - 1)) \\ & (17 + 8(k + 1), 26 + 8(k - 1)) \\ & (16 + 8(k + 1), 23 + 8(k - 1)) \\ & (21 + 8(k + 1), 30 + 8(k - 1)) \end{aligned}$$

Furthermore, $a_{i(i+1)} = 1$, for all integers i such that $1 \leq i \leq n - 1$ and $i \neq 14 + 8(k - 1); 1 \leq k \leq m$. Since the adjacency matrix of a graph is symmetric and all entries on the main diagonal is zero, our process completes our calculations for the adjacency matrix of $M(3, n)$. In Table 2., some pairs for which the corresponding entries of the adjacency matrix is one are given. We have also written the matrix $B_{22 \times 22}$ as an example.

Table 2. Some entries whose values in the adjacency matrix are equal to 1.

(1,14)	(4,13)	(12,20)	(6,11)	(10,18)	(9,15)	(14,22)
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- [7] Wolfram Research, Inc., Mathematica, Version 13.1, Wolfram Research, Inc., Champaign, Illinois, 2022.

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