STUDIA UBB. CHEMIA, LV, 4, 2010

KEKULÉ COUNT IN $TUC_4C_8(R)$ NANOTUBES

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ABSTRACT. Counting Kekulé structures is a very difficult problem in chemical graph theory. Some recent techniques allowed to estimate the lower bound of this number in certain classes of graphs. In this note a formula for the number of Kekulé structures in $TUC_4C_8(R)$ nanotube is given.

Keywords: *$TUC_4C_8(R)$ nanotube, Kekulé structure.*

INTRODUCTION

Kekulé structures (perfect matchings in graph theory) in benzenoid hydrocarbons are discussed in the famous book of Cyvin and Gutman [1]. In physics, the enumeration of Kekulé structures is equivalent to the dimer problem of rectangle lattice graph in the plane [2]. The Kekulé count of nanostructures has become interesting subjects of research. Close formulas for the Kekulé count have been obtained in [3-6].

A graph G consist of a set of vertices V(G) and a set of edges E(G). In chemical graphs the vertices of the graph correspond to the atoms of the molecule and the edges represent the chemical bonds. The number of vertices and edges in a graph will be denoted by |V(G)| and |E(G)|, respectively.

A matching of a graph G is a set M of edges of G such that no two edges of M share an end-vertex; further a matching M of G is perfect if any vertex of G is incident with an edge of M. The concept of perfect matching in graphs coincides with the Kekulé structure in organic chemistry. In this paper we focus our attention on the number of Kekulé structures in $TUC_4C_8(R)$ nanotube and a close formula is established, see [7-15] for details.

A C_4C_8 net is a trivalent decoration made by alternating rhombi C_4 and octagons C_8. It can cover either a cylinder or a torus. In some research papers, some topological indices of $TUC_4C_8(R/S)$ nanotubes and $TC_4C_8(R/S)$ nanotori have been investigated [16-22].

In this paper the $TUC_4C_8(R)[p,q]$ = TU[p,q] nanotube is considered, where p and q are the number of octagons in each row and column, respectively. We explain the methods for computing the number of Kekulé structures in TU[p,q] and compute exact formula for the number of Kekulé structures in

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some special case of $TUC_4C_8(R)$ nanotubes, see Figure 1 (notice that the edges in the left side are affixed to the vertex in the right side of the figure to gain a tube in this way).

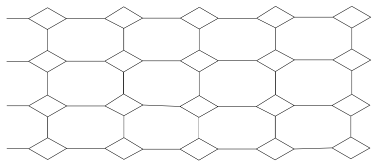

Figure 1. The chemical graph of TU[5,3].

MAIN RESULTS AND DISCUSSION

The aim of this section is to compute the number of Kekulé structures in TU[p,q] = $TUC_4C_8(R)$[p,q] nanotubes. The edges of rhombus in the molecular graph of TU[p,q] are called the rhomboidal edges while the other edges are named octagonal.

LEMMA 1. Consider the molecular graph of TU[p,1] = $TUC_4C_8(R)$[p,1] and E is a Kekulé structure of TU[p,1] containing a horizontal edge, Figure 2. Then c, d $\notin$ E and a, b $\in$ E.

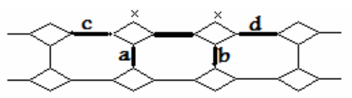

Figure 2. The molecular graph of TU[4,1].

PROOF. If E contains one of c or d then vertices shown by (x) could not be select in the matching, a contradiction. So, we must have the following figure for the matching:

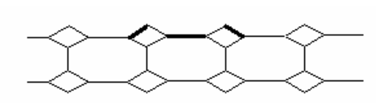

Figure 3. A part of a Kekulé structure without edges c and d.

By considering Figure 3 and the fact that in the upper selected rhomb, all the vertices must be covered, we have the following scheme for our Kekulé structure:

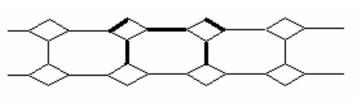

Figure 4. A part of a Kekulé structure containing a horizontal edge.

This completes our argument. ▲

Corollary. There are exactly two Kekulé structure containing a given horizontal edge. These are as follows:

Figure 5. A part of two possible Kekulé structures containing a horizontal edge.

Theorem 1. Suppose K(p,1) denotes the number of Kekulé structures in a TU[p,1] nanotube. Then we have:

$$K(p,1) = \begin{cases} 2^{2p} + p(2^{2p-4} + 2^{2p-8} + ... + 2^4) + 4 & p \, is \, even \\ 2^{2p} + p(2^{2p-4} + 2^{2p-8} + ... + 2^2) & p \, is \, odd \end{cases}$$

Proof. We first note there are 2^{2p} Kekulé structures when we consider only the rhomboidal edges of TU = TU[p,1], see Figure 6.

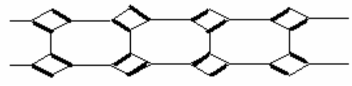

Figure 6. Kekulé structure containing rhomboidal edges.

Clearly, each of the rhomboidal edge can take part to a Kekulé structure in two schemes. Since the number of rhombi is 2p, we have 2^{2p} different choice for the number of Kekulé structures.

We now apply Lemma 1, to enumerate the Kekulé structures containing at least one non-rhomboidal edge.

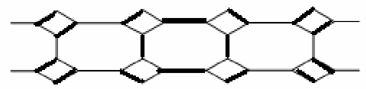

Figure 7. A Kekulé structure containing non-rhomboidal edges.

As it is shown in Figure 7, we have 2p − 4 rhombi, each of them belonging to two Kekulé structures and it is worth mentioning that this scheme can circulate in p situations. So, in this case we have $p2^{2p-4}$ Kekulé structures. Figure 8 shows a Kekulé structure when two of the octagonal edges in a row take part in matching. By lemma 1, we know that no two incident edges in a row may belong to a Kekulé structure.

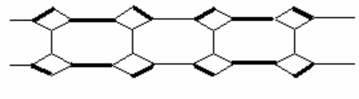

Figure 8. A Kekulé structure containing two of non-rhomboidal edges in a row.

At the end, we have a chain (Figure 9) that has two circulations for each of them. So we have 4 extra Kekulé structures, when p is even.

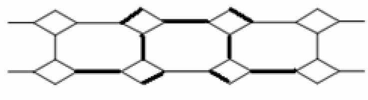

Figure 9. The extra Kekulé structures, when p is even.

This completes our proof. ▲

Using a similar argument as Theorem 1, one can compute the number of Kekulé structures of TU[2,q].

Theorem 2. The number of Kekulé structure in TU[2,q] is 4×5^q.

Proof. To calculate the number of Kekulé structure in TU[2,q], we first find a recursive equation for the number of Kekulé structures and then solve it. Suppose A(q) denotes the set of all Kekulé structures of TU[2,q] and x_q is its size. From Figure 10, one can see that there are two types of Kekulé structures for TU[2,q] as follows: the first type Kekulé structures contain both e_1 and f_1; the second type Kekulé structures are those without e_1 and f_1.

Suppose L_1 and L_2 denote the number of Kekulé structures of the first and second types, respectively. Then from Figure 10, it can easily seen that $L_1 = 4x_{q-1}$. Suppose M is a Kekulé structure of the second type. Also, there are $4x_{q-2}$ Kekulé structures of the second type such that $e_2,f_2 \notin M$. Continue this argument, we can see that $x_q = 4[x_{q-1} + x_{q-2} + \dots + x_1]$. To complete the proof, we must solve this recursive equation. To do this, notice that $x_{q-1} = 4[x_{q-2} + x_{q-3} + \dots + x_1]$ and so $x_q - x_{q-1} = 4\, x_{q-1}$. Therefore, $x_q = 5 \times x_{q-1}$ which implies that $x_q = 5^{q-1}\times x_1$. An easy calculation shows that $x_1 = 20$ and so $x_q = 4 \times 5^q$. ▲

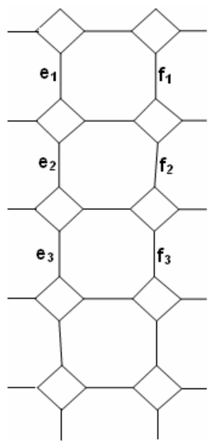

Figure 10. The Molecular Graph of TU[2,q].

From Theorems 1 and 2, we can find an upper and lower bounds for the number of Kekulé structures of TU[p,q] as follows:

Theorem 3. $(4\times 5^q)^{p/2} \le K(p,q) \le (4\times 5^q)^p$.

CONCLUSIONS

In this paper a simple method enabling to compute the Kekulé structures of $TUC_4C_8(R)$ nanotubes with a small number of rows or columns was presented. By this method an upper and lower bound for this number is also calculated. It is possible to extend our method in view of obtaining better bounds.

ACKNOWLEDGMENTS

The authors are indebted to the referee for some critical suggestions leaded us to correct our main result. This work was partially supported by the Nanoscience and Nanotechnology Research Center of the University of Tehran (Grant No. 6103007).

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