Iranian Journal of Mathematical Chemistry, Vol. 2, No.1, September 2011, pp. 53 - 59

IJMC

The Clar Number of Fullerene C_{24n} and Carbon Nanocone $CNC_4[n]$

MODJTABA GHORBANI• AND EHTERAM NASERPOUR

Department of Mathematics, Faculty of Science, Shahid Rajaee Teacher Training University, Tehran, 16785 – 136, I. R. Iran

(*Received June 1,* 2011)

ABSTRACT

A fullerene graph is a 3−connected planar graph whose faces are pentagons and hexagons. The Clar number of a fullerene is the maximum size of sextet patterns, the sets of disjoint hexagons which are all *M*-alternating for a Kekulé structure *M* of *F*. An exact formula of Clar number of some fullerene graphs and a class of carbon nanocones are obtained in this paper.

Keywords: Fullerene, Clar number, Sextet pattern, Carbon nanotube, Kekulé structure.

1. INTRODUCTION

In the past years, nanostructures involving carbon have been the focus of an intense research activity which is driven to a large extent by the quest for new materials with specific applications. Fullerene is one of the main objects of nanostructures. A fullerene is any molecule composed entirely of carbon, in the form of a hollow sphere, ellipsoid, or tube. Spherical fullerenes are also called buckyballs and cylindrical ones are called carbon nanotubes or buckytubes. Fullerenes are similar in structure to graphite, which is composed of stacked graphene sheets of linked hexagonal rings; but they may also contain pentagonal rings. By Euler's theorem, one can prove the number of pentagons and hexagons in a fullerene molecule C_n are 12 and $n/2 - 10$, respectively. The first fullerene to be discovered, and the family's namesake, was buckminsterfullerene C_{60}, made in 1985 by Robert Curl, Harold Kroto and Richard Smalley [1–3].

•*Corresponding author* (*Email: mghorbani@srttu.edu*).

For a given graph *G*, a matching *M* in *G* is a set of pair wise non−adjacent edges; that is, no two edges share a common vertex. A matching *M* of a graph *G* is maximal if every edge in *G* has a non−empty intersection with at least one edge in *M*. A matching *M* is perfect if all vertices are matched by *M*. A Kekulé structure (perfect matching in graph theory) of a fullerene graph *F* is a set of independent edges covering all vertices. The edges in a Kekulé structure are illustrated by double bonds. A set *S* of disjoint hexagons of *F* is called a sextet pattern if *F* has a Kekulé structure such that every hexagon in *S* contains three double bonds or equivalently if the deletion of the hexagons in *S* together with their incident edges results in a subgraph of *F* with a Kekulé structure. A sextet pattern of *F* with the maximum number of hexagons is called a Clar formula or Clar structure. The number of hexagons in any Clar formula is called the Clar number of a fullerene *F*. In Clar's model [4], a sextet pattern *S* is designated by depicting circles within hexagons of *S,* Figure 1.

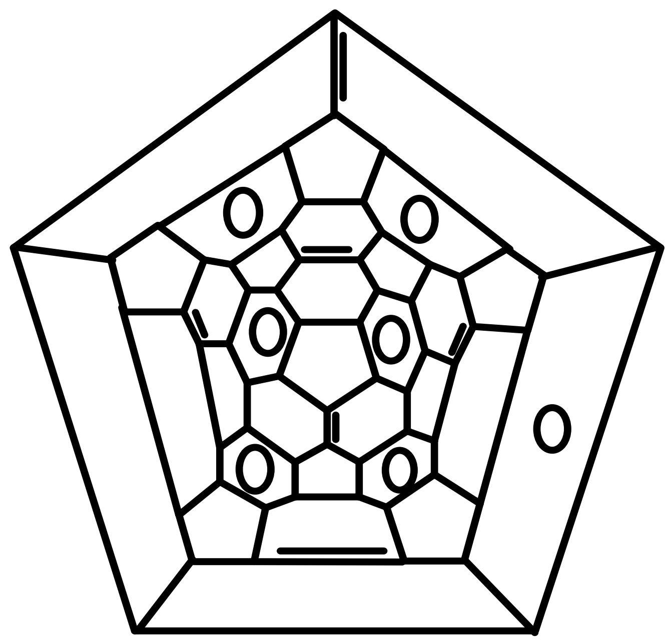

Figure 1. The Clar Formulas of Icosahedral C_{60}.

The concept of resonant pattern originates from Clar's aromatic theory [4]: within benzenoid hydrocarbon isomers, one with larger Clar number is more stable. Some upper bounds for the Clar number of benzenoid hydrocarbons, were given by Hansen and Zheng [5].

2. RESULTS AND DISCUSSIONS

In this section we compute the Clar number of two classes of nanostructures, namely an infinite class of fullerenes with 24*n* vertices and a class of tetragonal carbon nanocone.

In [6] a method is described to obtain a fullerene graph from a zig–zag or armchair nanotubes. Here by continuing this method we construct an infinite class of fullerenes and then we obtain its Clar number. Denoted by $T_Z[q, p]$ means a zig–zag nanotube with p rows and q columns of hexagons, Figure 2. Combine a nanotube $T_Z[12, p]$ with two copies of caps B, Figure 3,as shown in Figure 4, the resulted graph is a IPR fullerene, which has $24n$ vertices and exactly $12n – 10$ hexagonal faces. In this section we compute the Clar number of this fullerene. To do this, we should to calculate the Clar number of $T_Z[12, p]$ nanotube. In the following theorem this value is computed:

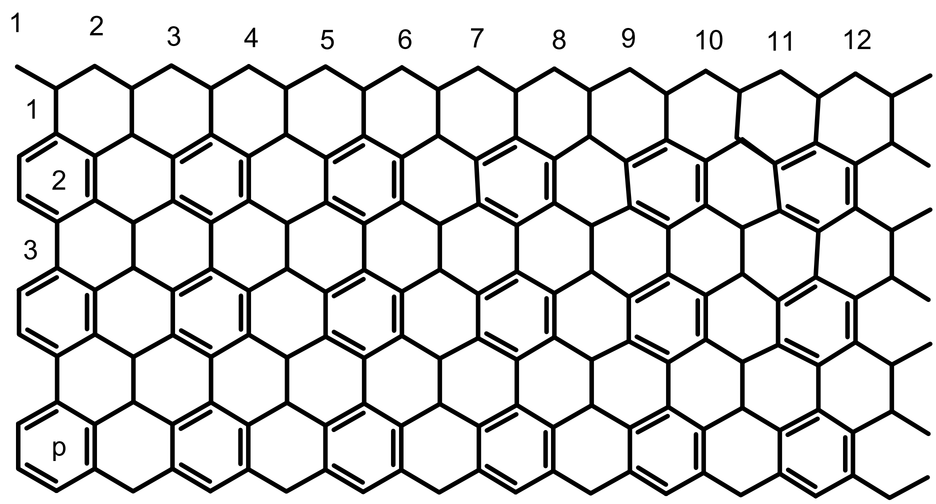

Figure 2. The 2D Graph of Zig–Zag Nanotube $T_z[12,p]$,
for $p = 6$ and its Clar Structures.

Theorem 1. Consider a nanotube $T_Z[12, p]$ with p rows and 12 columns. Then its Clar number is:

$$m(T_Z[12, p]) = 6\lceil p/2 \rceil.$$

Proof. At first consider the zig–zag nanotube $T_Z[12, p]$ as depicted in Figure 2. The number of resonant hexagons in each row is 6. Consider two following cases:

1) p is odd, in this case the number of resonant hexagons in the nanotube $T_Z[12, p]$ is $6(p+1)/2$.
2) p is even, in this case the number of resonant hexagons is $6p/2$ and this completes the proof.

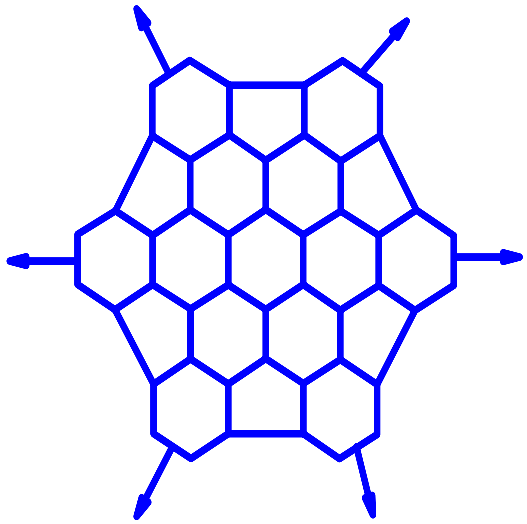

Figure 3. The Cap B.

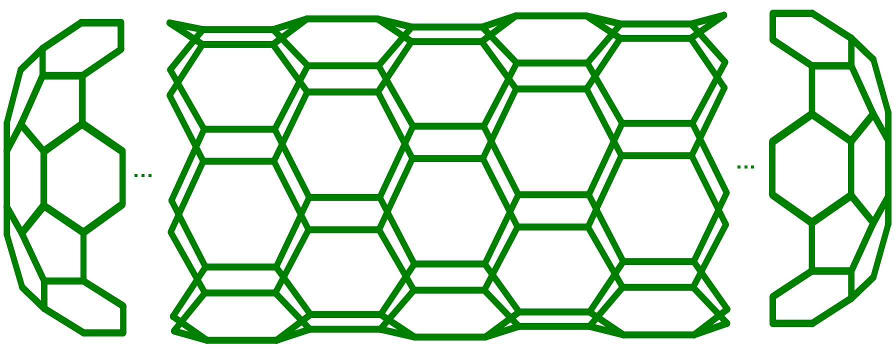

Figure 4. Fullerene C_{24n} Constructed by Combining two Copies of Cap B and the Zig–Zag Nanotube $T_Z[12, p]$.

Corollary 2. The Clar number of fullerene C_{24n} is as follows:

$$m(C_{24n}) = \begin{cases} 3n+1 & 2 \nmid n \\ 3n+2 & 2 \mid n \end{cases}.$$

Proof. Combine a nanotube $T_Z[12, n\text{-}3]$ with two copies of caps B, see Figure 4. To complete the proof we consider two cases:

1. n is even. In this case the number of resonant hexagons in $T_Z[12 , n - 3]$ is $6[(n-3)/2] = 3(n-4)$ and the total number of resonant hexagons in both caps are 14. So, the Clar number of fullerene C_{24n} in this case is $3n + 2$.

2. n is odd. In this case the number of resonant hexagons in the nanotube $T_Z[12, n-3]$ is $6[(n-3)/2] = 3(n-3)$, the number of total resonant hexagons in both caps are 10 and this prove the second claim.

Carbon nanocones are structures which are made from carbon and which have at least one dimension of the order equal or less than one micrometer. Nanocones occur on the surface of natural graphite. In the final section of this paper we compute the Clar number of a tetragonal carbon nanocones NCN[4, n], depicted in Figure 5.

Let n be the number of hexagonal layers around the central tetragon. We can put a circle in two hexagons in the first layer of hexagons, as depicted in Figure 5. For the second layer we can put again four circles, but this value is 6 for the third layer. By continuing this method, one can see that the numbers of circles in the n^{th} layer, $n > 2$, are 2, 2, 4, 6, 6, 8, 10, 10 and so on. In other words, if $\eta(CNC[4,n])$ be the number of circles in the n^{th} layer ($n > 2$), then we have:

$$\eta(CNC[4,n]) = \left[\frac{2n+1}{3}\right].$$

This implies that the Clar number of carbon nanocones CNC[4,n] can be computed as follows:

i) $n \equiv 0 (\text{mod } 3)$, in this case we have

$$m\left(CNC_4[n]\right) = 2\left(1+1+2+\ldots+[\frac{2n-1}{3}]+[\frac{2n-1}{3}]+[\frac{2n+1}{3}]\right)$$
$$= 2\left(1+2+3+\ldots+[\frac{2n+1}{3}]\right)+2\left(1+3+\ldots+[\frac{2n-1}{3}]\right)$$
$$= 2\left(\frac{[\frac{2n+1}{3}]([\frac{2n+1}{3}]+1)}{2}+(\frac{n}{3})^2\right).$$

ii) $n \equiv 1 (\text{mod } 3)$, in this case one can see that

$$m\left(CNC_4[n]\right) = 2\left(1+1+2+\ldots+[\frac{2n-3}{3}]+[\frac{2n-1}{3}]+[\frac{2n+1}{3}]\right)$$
$$= 2\left(1+2+3+\ldots+[\frac{2n+1}{3}]\right)+2\left(1+3+\ldots+[\frac{2n-3}{3}]\right)$$
$$= 2\left(\frac{[\frac{2n+1}{3}]([\frac{2n+1}{3}]+1)}{2}+[\frac{n}{3}]^2\right).$$

iii) $n \equiv 1 (\text{mod } 3)$, in this case we can prove that

$$m(CNC_4[n]) = 2\left(1+1+2+\ldots+[\frac{2n-3}{3}]+[\frac{2n+1}{3}]+[\frac{2n+1}{3}]\right)$$
$$= 2\left(1+2+3+\ldots+[\frac{2n+1}{3}]\right)+2\left(1+3+\ldots+[\frac{2n+1}{3}]\right)$$
$$= 2\left(\frac{[\frac{2n+1}{3}]([\frac{2n+1}{3}]+1)}{2}+\left\lceil\frac{n}{3}\right\rceil^2\right).$$

So, we proved the following Theorem:

Theorem 5. Consider a carbon nanocones CNC[4, n]. Then its Clar number is as follows:

$$m(G)=\begin{cases} 2\left(\frac{[(2n+1)/3]([(2n+1)/3]+1)}{2}+(n/3)^2\right) & 3\mid n \\ 2\left(\frac{[(2n+1)/3]([(2n+1)/3]+1)}{2}+\lceil n/3\rceil^2\right) & 3\mid n-1 \\ 2\left(\frac{[(2n+1)/3]([(2n+1)/3]+1)}{2}+\lceil n/3\rceil^2\right) & 3\mid n-2 \end{cases}.$$

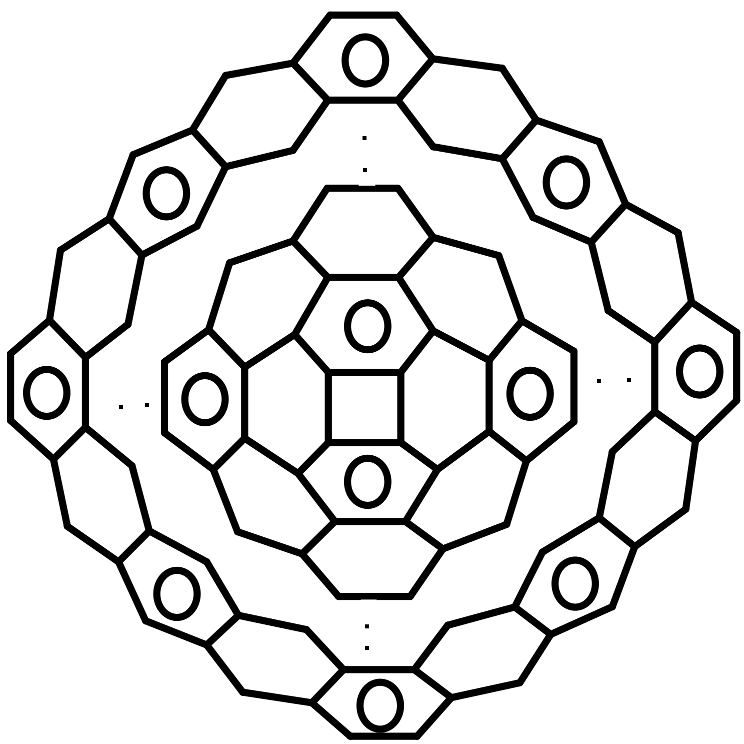

Figure 5. The 2D Graph of Carbon Nanonocone CNC[4,3].

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