OPTOELECTRONICS AND ADVANCED MATERIALS – RAPID COMMUNICATIONS Vol. 4, No. 8 August 2010, p. 1261 - 1263

Non – commuting graphs of group automorphism of an infinite family of fullerenes

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Let G be a non-abelian group and let $Z(G)$ be the center of G. We associate with G a graph Γ_G as follows: Take $G\backslash Z(G)$ as vertices of Γ_G and join two distinct vertices x and y whenever $xy \neq yx$. The graph Γ_G is called the non-commuting graph of G. In this paper we compute non – commuting graph of dihedral group D_{2n} as a symmetry group of some fullerene graphs.

(Received July 20, 2010; accepted August 12, 2010)

Keywords: Fullerene, Non – commuting graphs, Conjugacy classes, Dihedral group

1. Introduction

A graph is a collection of points and lines connecting them. The points and lines of a graph are called vertices and edges respectively. If e is an edge of G, connecting the vertices u and v, then we write $e = uv$ and say "u and v are adjacent". A connected graph is a graph such that there exists a path between all pairs of vertices.

Mathematical calculations are absolutely necessary to explore important concepts in chemistry. Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is an important tool for studying molecular structures. This theory had an important effect on the development of the chemical sciences. 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.

Fullerenes are carbon-cage molecules in which a large number of carbon (C) atoms are bonded in a nearly spherically symmetric configuration, which was discovered for the first time in 1985 [1]. Let p, h, n, and m be the number of pentagons, hexagons, carbon atoms and bonds between them, in a given fullerene F. Since each atom lies in exactly 3 faces and each edge lies in 2 faces, the number of atoms is $n = (5p+6h)/3$, the number of edges is $m = (5p+6h)/2 = 3/2n$ and the number of faces is $f = p + h$. By the Euler's formula $n - m + f = 2$, one can deduce that $(5p + 6h)/3 - (5p+6h)/2 + p + h = 2$, and therefore $p = 12$, $v = 2h + 20$ and $e = 3h + 30$. This implies that such molecules made up entirely of n carbon atoms and having 12 pentagonal and $(n/2 - 10)$ hexagonal faces, where $n \neq 22$ is a natural number equal or greater than 20 [2,3].

We now recall some algebraic definitions that will be used in the paper. Throughout this paper, graph means simple connected graph. The vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. If x and y are two vertices of G then $d(x,y)$ denotes the length of a minimal path connecting x and y. A topological index for G is a numeric quantity that is invariant under automorphisms of G. A distance-counting polynomial was introduced by Hosoya [2, 3] as $H(G,x) = \sum_k d(G,k)x^k$. The Wiener index of a graph G, named after the chemist Harold Wiener [4], who considered it in connection with paraffin boiling points, is given by $\frac{1}{2}\sum_{x,y\in V(G)} d_G(x,y)$, where d_G denotes the distance in G. Besides its purely graph-theoretic value, the Wiener index has interesting applications in chemistry.

Let G be a non-abelian group and let $Z(G)$ be the center of G. We associate with G a graph Γ_G as follows: take $G\backslash Z(G)$ as vertices of Γ_G and join two distinct vertices x and y whenever $xy \neq yx$. The graph Γ_G is called the non-commuting graph of G. Many graph theoretical properties of Γ_G is studied in [5-10].

2. Main results

Groups are often used to describe symmetries of objects. This is formalized by the notion of a group action. A symmetry group is a group of symmetry-preserving operations, i.e., rotations, reflections, and inversions. In mathematics, the symmetric group on a set is the group consisting of all bijections of the set with the composite function as the group operation.

The dihedral group D_{2n} is the symmetry group [12-22] of an n-sided regular polygon for $n > 1$. These groups are one of the most important classes of finite groups currently applicable in chemistry. For example the point groups D_3, D_4, D_5 and D_6 are dihedral groups. A group presentation for D_{2n} is $\langle x,y \mid x^n = y^2 = e, yxy = x^{-1}\rangle$.

Lemma 1. The automorphism group of graph fullerene C_{10n} (Fig. 1) is isomorphic with dihedral group D_{20}.

Proof. Consider the Graph of Fullerene C_{10n} in Fig. 1. By using symmetry concept, one can see that the generators of this group are:

$\sigma = (2,5)(3,4)(6,10)(7,9)(11,15)(12,14)...(10n-4,10n)(10n-3,10n-1)$,

where fixed elements are

$$1,8,19,30,\ldots,11i\text{-}3,11i+2,\ \ldots,10n\text{-}2(i=1,2,\ldots,n\text{-}1)$$

and

$$\tau = (1,10n-4,2,10n-3,3,10n-2,4,10n-1,5,10n)....$$
$$(7,10n-6,9,10n-14,11,10n-12,13,10n-10,15,10n-8)$$

Now by using GAP[23] we can see that the group generated by σ and τ is isomorphic to D_{20}.

It is easy to see that the non – commuting graph of symmetry group of fullerene C_{10n}, has ten vertices of degree 18 and nine vertices of degree 10. In general we have the following Theorem:

Theorem 3. Non – commuting graph of group D_{2n} is as follows:

i) if n is odd, then $\Gamma_G \cong H$, where H has exactly n vertices of degree $2n$ -2 and n-1 vertices of degree n,

ii) if n is even, then $\Gamma_G \cong K$, where K has exactly n vertices of degree $2n$ – 4 and n-2 vertices of degree n,

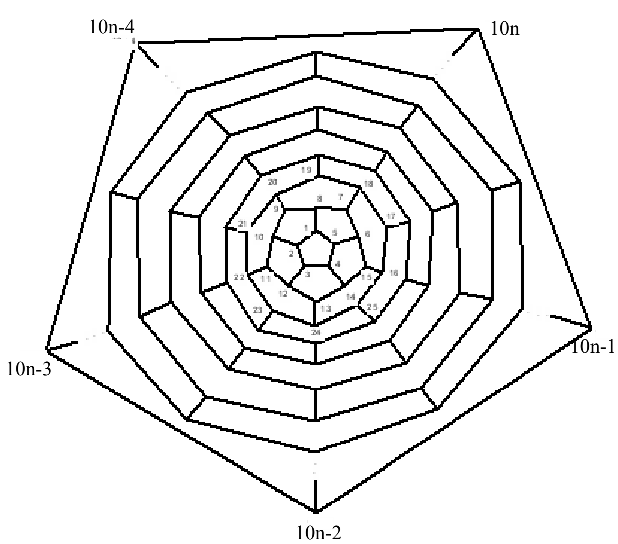

Fig. 1. Graph of Fullerene C_{10n}.

Proof. We know that D_{2n} is $<x,y \mid x^n = y^2 = e, yxy = x^{-1}>$. Let n be odd. So $Z(D_{2n}) =\{e\}$ and $C_G(yx^i)=\{e, y x^i\}$, for $i = 0,1,\ldots,n$-1. Also $C_G(x^i)=<x>$, for i=1,2,…n-1. Thus, by the definition of non-commuting graph of group, $deg(yx^i) = |G\text{-}\{e, y x^i\}|=2n\text{-}2$, for $i = 0,1,\ldots,n\text{-}1$ and $deg(x^i)=|G\text{-}<x>|=2n - n = n$.

Now let n be even. Thus $Z(D_{2n})=\{e, x^{n/2}\}$ and so $C_G(yx^i)=\{e, y x^i, x^{n/2}, yx^{i+n/2}\}$, where i=0,1,…,n-1 and $C_G(x^i)=<x>$, for i=1,2,…n/2-1, n/2+1,…n-1. Therefore $deg(yx^i)=|G\text{-}\{e, y x^i, , x^{n/2}, yx^{i+n/2}\}|=2n\text{-}4$, for i=0,1,…,n-1 and $deg(x^i)=|G\text{-}<x>|=2n\text{-}n = n$ >, for i=1,2,…n/2-1, n/2+1,…n-1.

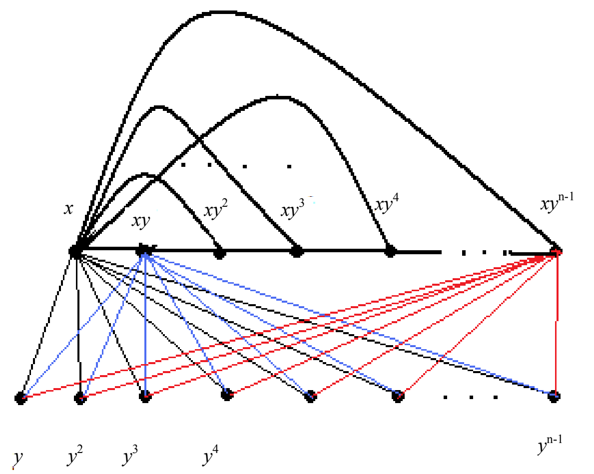

Fig. 2. Non – commuting graph of group D_{2n}., where n is odd.

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