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Group Autormorphism of Some Fullerenes and Prime Graph

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ABSTRACT

Let G be a finite Group and *π (G)* be the set of prime numbers that divide the |*G*|. We associate with *G* a graph V_G as follows : Take *π (G)* as vertices of V_G and join two distinct vertices *p* and *q* if there is an element $g \in G$ with *o(g)=pq*. This graph is named prime graph of *G* and in this paper we computer prime graph of dihedral group D_{2n} as a symmetry group of same Fullerene graphs.

Keywords: *Fullerene, Prime graph. Dihedral group.*

1. INTRODUCTION

A graph G is a binary G = (V,E) that V is the points and E is the 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 pair vertices.

Mathematical calculation is absolutely necessary to explore important concepts in chemistry. Mathematical chemistry is a branch of theoretical chemistry for discussion and predication 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 active 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 I 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 atomic 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 edge is $m = (5p + 6h)/2 = 3/2n$ and the number of faces i $f = p + h$ s. by the Euler's formula $n - m + f = 2$, one can daduce that $\frac{(5p+6h)}{3} - \frac{5p+6h}{2} + p + h = 2$, and therefore $p = 12$, $v = 2h + 20$ and $e = 3h + 30$. This implies that such molecules made up entirely for n carbon atoms and having 12 pentagonal and $({}^{n}/_{2} - 10)$ hexagonal faces, where $n \neq 22$ is a natural number equal or grater than 20 [2,3].

We now recall same algebraic definitions that will be used in the paper. Throughout this paper, graph means simple graph without any loop. The vertex and edge sets of a graph G denoted by V(G) and E(G), respectively. If x and y are two vertices of G the d(x,y) denotes the length of minimal path connecting x and y. A topological index for G is numeric quantity that is invariant under automorphism 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 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. In [18] some topological indexes of same molecular graph were computed.

Let G be a finite group and $\pi(G)$ be the set of prime number that divide |G|. The prime graph ∇_G associate with G as follows: take $\pi(G)$ as vertices of ∇_G and join two distinct vertices p and q whenever there is an element g∈G with $o(g) = pq$ that o (g) is the order of g. Many graph theoretical properties of $\nabla_G$is studied in [5-8].

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2. MAIN RESULTS

Symmetries of objects are often described by groups. This is formulized by the notion of group action. A Symmetry group is a group of group Symmetry-preserving operation, i.e. rotations, reflection and inversions. In mathematics, the Symmetric group of 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 [9-17] 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:

$< x, y | x^n = y^2 = e, yxy = x^{-1} >$

Lemma 1:

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

Proof:

If we consider the graph of fullerene C_{10n} in Fig.1, then by using the symmetry concept see that he 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

$1,8,19,30, \dots ,11i-3,11i+2, \dots ,10n-2 \quad (i = 1,2, \dots, n-1)$

and

$\tau = (1,10-4,2,10n-3,3,10n-2,4,10n-1,5,10n) \dots$

$(7,10n-6,9,10n-14,11,10n-12,10n-10,15,10n-8)$

Now by using GAP[19] we can see that the group generated by τ and σ is isomorphic to D_{2O}.

In the following we distinguish the structure of prime graph of D_{2n}.

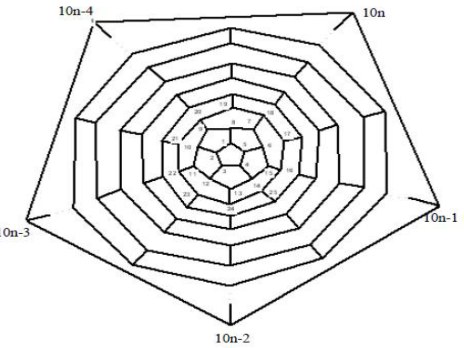

Fig 1: Graph of fullerene C_{10n}

Theorem 2:

If $n = P_1^{\alpha_1} P_2^{\alpha_2} \dots P_s^{\alpha_s}$ for distinct prime numbers P_i and positive integers α_i $(i = 1,2, \dots, s)$, then the prime graph of group D_{2n} as follows:

i) If n is even, then it is a complete graph with s vertices.

ii) If n is odd, then it is not connected, with a single vertex and s vertices of degree s-1.

Proof:

We know that D_{2n} = $< x, y | x^n = y^2 = e, yxy = x^{-1} > =$ $\{e, y, x, x^2, \dots, x^{n-1}, yx, yx^2, \dots, yx^{n-1}\}$

Let n be even and we may assume that $p_1 = 2$. If p_i and p_j are distinct prime numbers that $p_i | n$ and $p_j | n$, then we have $(x^{\frac{n}{p_i p_j}})^{p_i p_j} = e$. so $o(x^{\frac{n}{p_i p_j}})$=$p_i p_j$ that means p_i is joined to p_j in prime graph of D_{2n}. Therefore any two prime divisor of n are joined, will result the prime graph is a complete graph with s vertices.

Let n be odd. So $Z(D_{2n}) = \{e\}$ and for any $yx^r (r = 1,2, \dots, n-1)$, we deduce that $o(yx^r) = 2$. also for any $x^t (t = 1, \dots, n-1)$, we have $(x^t)^n = e$ and so $o(x^t) | n$ which means $o(x^t)$ is an odd. By the same proof to case n even, we have any two distinct odd prime p_i and p_j are adjacent. So the vertex 2 is single and the others vertices are joined together, the proof is completed.

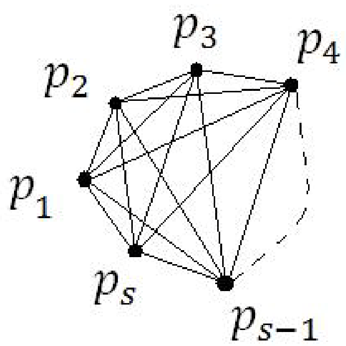

Fig 2: K_s as a prime graph for D_{2n}, when n is odd

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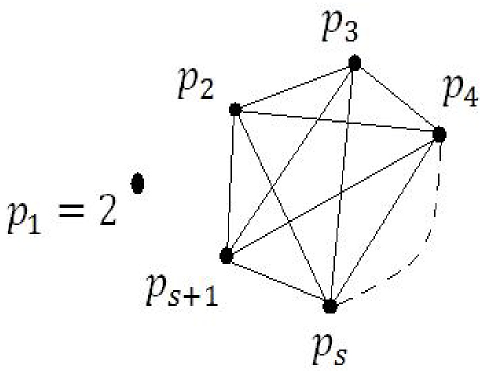

Fig 3: $(k_1 \cup k_s)$ As a prime graph for $D_{2n,}$ when n is even

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