Applied Mathematics and Computation 282 (2016) 237–243

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

On the automorphism group of polyhedral graphs

Modjtaba Ghorbani*, Mahin Songhori

Department of Mathematics, Faculty of Science, Shahid Rajaee, Teacher Training University, Tehran 16785-136, Islamic Republic of Iran

A R T I C L E   I N F O

Keywords:
Fullerene
Group action
Stabilizer
Automorphism group

A B S T R A C T

A (4,6)-fullerene is a three connected cubic planar graph whose faces are squares and hexagons. In this paper, for a given (4,6)-fullerene graph F, we compute the order of automorphism group F. We also study some spectral properties of fullerene graphs via their automorphism group.

1. Introduction

A ***graph*** is a collection of points and lines connecting them. Let us to call these points and lines by vertices and edges, respectively. Two vertices x and y are adjacent, if $e = uv$ is an edge of the graph. A graph whose any vertex pair is connected by a path is called a connected graph. A simple graph is a graph without loop and parallel edges. The vertex and edge-sets of the graph G are represented by $V(G)$ and $E(G)$, respectively. A ***molecular graph*** (chemical graph) is a labeled simple graph whose vertices and edges correspond to the atoms and chemical bonds, respectively. Its vertices are labeled with the kinds of the corresponding atoms and edges are labeled with the types of bonds, [1]. In a molecular graph, it is convenient to omit hydrogen atoms.

By using methods of graph theory, we can construct cubic graphs whose faces have the size r and 6, to satisfy Euler's formula for $r \in \{3,4,5\}$. The most important fullerenes are (5,6) fullerenes discovered by Kroto and his team in 1985, see [18,19]. There are many problems concerning with fullerene graphs and many properties of them are studied by mathematician, see [1,2,4–8,10–12,15–17,20–22]. Among other classes of fullerene graphs, (4,6) fullerenes play a significant role in the study of fullerenes. In general, a (4,6)-fullerene is a cubic planar graph whose faces are squares and hexagons. Such fullerenes are sometimes called (4,6)-cages. Let s, h, n and m be the number of squares, 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 $n = (4s + 6h)/3$, the number of edges is $m = (4s+6h)/2 = 3/2n$ and the number of faces is $f = s+h$. By the Euler's formula $n - m+f = 2$, one can deduce that $(4s + 6h)/3 - (4s + 6h)/2+s+h = 2$, and therefore $s = 6$, $n = 2h+8$ and $m = 3h+12$. This implies that such molecules are made entirely of n carbon atoms and have six squares and $(n/2 - 4)$ hexagonal faces where n is an even non-negative integer.

The smallest (4,6) fullerene is a cube or hexahedron, see Fig. 1. It is composed of six squares, three of which meet at each vertex. It has twelve edges and eight vertices. The symmetry group of tetrahedron is isomorphic to $\mathbb{Z}_2 \times S_4$.

An automorphism of the graph $\Gamma = (V, E)$ is a bijection σ on V which preserves the edge set E, if $e = uv$ is an edge, then $\sigma(e) = \sigma(u)\sigma(v)$ is an edge of E. Here, the image of vertex u is denoted by $\sigma(u)$. The set of all automorphisms of a graph Γ with the operation of composition of permutations is a permutation group on $V(\Gamma)$denoted by $Aut(\Gamma)$.

* Corresponding author. Tel./fax: +98 2122970005.
E-mail address: mghorbani@srttu.edu, ghorbani30@gmail.com (M. Ghorbani).

http://dx.doi.org/10.1016/j.amc.2016.01.066

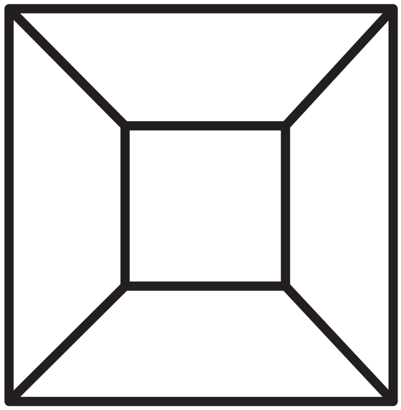

Fig. 1. 2-D graph of the cube.

The paper is organized as follows: In Section 2 notions concerning this paper are introduced together with the notation. Here, our notations are standard and mainly taken from [3,9,13]. Section 3 is devoted to proving Theorem 5 and then some new results on the automorphism group of a fullerene graph with respect to their graph spectrum are proposed.

2. Definitions and preliminaries

Groups are often used to describe symmetries of objects. This is formalized by the notion of a group action. Let G be a group and X a nonempty set. An action of G on X is denoted by $(G|X)$ and X is called a G-set. It induces a group homomorphism φ from G into the symmetric group S_X on X, where $\varphi(g)x = gx$ for all $x \in X$. The orbit of x will be denoted by x^G and is defined as the set of all x^g, $g \in G$. The degree of an action is the size of X. The kernel of the action is the kernel of φ and the action is faithful when Ker $\varphi = 1$. The stabilizer of element $x \in X$ is defined as

$$G_x = \{g \in G | g.x = x\}.$$

Let $H = G_x$ then for $x \neq y \in X$, H_y is denoted by $G_{x,y}$. On the other hand, the orbit-stabilizer theorem implies that, $|x^G|.|G_x| = |G|$. A group G acting on a set X is said to be transitive on X if it has only one orbit, and so $x^G = X$ for all $x \in X$. A group G acting transitively on a set X is said regularity, if $G_x = 1$ for all x in X. For every g in G, let $fix(g) = \{x \in X, g.x = x\}$, then we have:

Lemma 1. ***(Burnside).*** *Let G acts on the set X, then the number of orbits of G is*

$$\frac{1}{|G|}\sum_{g\in G}|fix(g)|.$$

The fullerenes described in this paper via their automorphism groups. The aim of this paper is to prove that the order of the automorphism group of a (4,6) fullerene divides 48. A semi-regular element of G is a nonidentity element having all cycles of equal length in its cycle decomposition. In particular, a (k,n)-semi-regular element of G is a non-identity element having k orbits of length n and no other orbit.

3. Main results

Fowler and his co-authors showed that fullerenes are realizable within 28 point groups [13]. In [21] Kutnar et al. proved that for any (5,6) fullerene graph F, $|\mathrm{Aut}(F)|$ divides 120. Ghorbani et al. [14] proved that for a (3,6) fullerene such as F, $|\mathrm{Aut}(F)|$ divides $2^3 \times 3$. Following their method, we compute the order of automorphism group of (4,6) fullerene graphs.

3.1. Relations between automorphism group of fullerenes and their spectrum

The adjacency matrix $A(G)$ of graph G with the vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ is an $n \times n$ symmetric matrix $[a_{ij}]$, such that $a_{ij} = 1$ if v_i and v_j are adjacent and 0, otherwise. The characteristic polynomial $\Phi(G, x)$ of graph G is defined as

$$\Phi(G, x) = \det(A(G) - xI).$$

The roots of the characteristic polynomial are the eigenvalues of graph G and form the spectrum of graph G.

In this section, we study some properties of the automorphism group of fullerene graphs with respect to their spectrum. We recall that a simple eigenvalue λ of graph G is that one whose multiplicity is 1 and thus a simple graph is one whose