STUDIA UBB CHEMIA, LXI, 1, 2016 (p. 243-248)
(RECOMMENDED CITATION)

Dedicated to Professor Mircea Diudea on the Occasion of His 65th Anniversary

ON (3,6) AND (4,6)–FULLERENE CAYLEY GRAPHS

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ABSTRACT. An (r, s)–fullerene graph is a planar 3–regular graph with only C_r and C_s faces, where C_n denotes a cycle of length n. In this paper the (3,6)–fullerene Cayley graphs constructed from finite groups are classified. A characterization of (4,6)–fullerene Cayley graphs is also presented.

***Keywords**: Fullerene, Cayley graph, finite group.*

INTRODUCTION

In this paper, the word graph refers to a finite, undirected graph without loops and multiple edges.

Let G be a group and S a subset of G not containing the identity element. We define the Cayley digraph X = Cay(G,S) of G with respect to S by V(X) = G and E(X) = {(g,gs) | $g \in G$, $s \in S$}. It is not so difficult to prove that X is undirected if and only if $S = S^{-1} = \{s^{-1} \mid s \in S\}$. In the latter case, we call X a Cayley graph.

The notion of a map satisfies the originally intuitive problem of "drawing a graph without intersections". Let us denote the group of all map–automorphism of M by *Aut(*M*)*. If *Aut(*M*)* contains a subgroup that acts regularly on the vertex set then M is called a Cayley map. Since $Aut(M) \leq Aut(X)$ we clearly have that the underlying graph X of a Cayley map is a Cayley graph. Equivalently,

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a Cayley map is an embedding of a Cayley graph onto an oriented surface having the same cyclic rotation of generators around each vertex. These are studied extensively in literature, see [1–3] for more details on this subject.

A graph which can be drawn in the plane in such a way that edges meet only at points corresponding to their common ends is called a planar graph. An (r,s)–fullerene graph is a planar 3–regular graph with only r– and s–faces, where an n–face is a face of size n. Suppose p, h, n and m are the number of r–faces, s–faces, vertices and edges, respectively, in a given (r,s)–fullerene, where (r,s) = (3,6);(4,6). Since each vertex in an (r,s)–fullerene graph lies in exactly 3 faces and each edge lies in 2 faces, the number of vertices is $n = (rp + sh)/3$, the number of edges is $m = (3/2)n = (rp + sh)/2$ and the number of faces is $f = p + h$. By the Euler's formula $n - m + f = 2$, one can deduce that $(rp + sh)/3 - (rp + sh)/2 + p + h = 2$, and therefore the number of 3–faces in (3,6)–fullerenes is four while the number of 4–faces in (4,6)–fullerenes is six. This implies that (3,6)–fullerenes have exactly four triangles and $n/2 - 2$ hexagons. Similarly, (4,6)–fullerenes have exactly 6 squares and $n/2 - 4$ hexagons. The (4,6)–fullerenes with isolated squares are called ISR–fullerenes. The name is taken from [4] in which the authors used the name IPR–fullerene for those with disjoint pentagons.

Computations were carried out by the aid of GAP [5]. The motivation for this study is outlined in [3,6–8] and the reader is encouraged to consult these papers for background material as well as for basic computational techniques. Our notation is standard and taken mainly from [4].

RESULTS AND DISCUSSION

Since the discovery of C_{60} fullerene in 1985 by Kroto *et al.*, the fullerenes became the subject of interest of scientists all over the world [9,10]. The aim of this section is to characterize the (3,6)– and (4,6)–fullerene Cayley graphs [11]. We begin by (3,6)–fullerene Cayley graphs.

Theorem 1. Let X = Cay(G,S) be a (3,6)–fullerene Cayley graph on a group G. Then, either G is isomorphic to an abelian group of order 4 and X is isomorphic to the complete graph K_4, or G is isomorphic to the alternating group A_4 and X is isomorphic to the graph shown in Figure 1.

Proof. By Euler's formula X contains a 3–cycle. Since X is cubic and undirected, then S is of cardinality 3 and $S=S^{-1}$. If S consists of three involutions a, b and c then a 3–cycle in X must arise from the relation abc = e, which implies that c = ab and consequently $G = \langle a, b, c\rangle = \langle a, b \mid a^2 = b^2 = (ab)^2 = e\rangle \cong Z_2 \times Z_2$

and $X \cong K_4$. If however S consists of an involution a, a non–involution x and the inverse of this non–involution then a 3–cycle in X arises either from the relation $x^3 = e$ or from the relation $x^2a = e$. In the former case the edge with end vertices e and x must lie on a 6–cycle arising from the relation $(ax)^3 = e$ and thus $G = \langle a, x \mid a^2 = x^3 = (ax)^3 = e\rangle \cong A_4$ and X is isomorphic to the graph shown in Figure 1. In the latter case $G = \langle x \mid x^4=e\rangle \cong Z_4$ and $X \cong K_4$. This completes our proof.

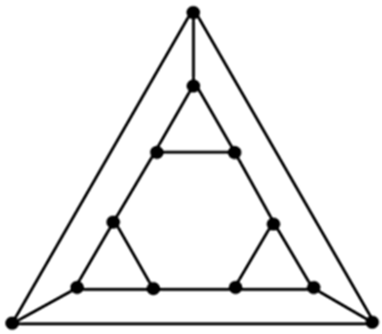

Figure 1. The (3,6)–fullerene Cayley graph on the alternating group A_4.

Theorem 2. Let X = Cay(G,S) be a (4,6)–fullerene Cayley graph on group G.

Then

I. G is isomorphic to the dihedral group D_8 or $Z_2 \times Z_4$ with a Cayley graph isomorphic to the cube Q_3,

II. G is a finite quotient of an infinite group H presented as follows:

$$H = \langle a, b, c \mid a^2 = b^2 = c^2 = e, (ab)^2 = e \rangle,$$

III. G is a finite quotient of the free product group $Z_2 \blacklozenge Z_2$,

IV. G is isomorphic to the symmetric group S_4 with a Cayley graph isomorphic to an ISR–fullerene on 24 vertices depicted in Figure 2,

V. G is isomorphic to the dihedral group D_{12} with a Cayley graph isomorphic to a 6–prism depicted in Figure 3,

VI. G is a finite quotient of an infinite group H isomorphic to an extension of $Z_2 \times Z_2$ by Z_2.

Proof. Suppose X = Cay(G,S) is a (4,6)–fullerene. Since X is 3–regular, we can assume that S = {a, b, c}. By similar argument as Theorem 1, we consider the following cases:

Case 1. $a^2 = b^2 = c^2 = e$. A tedious calculation shows that we can assume that the 4–face of X arise from $(ab)^2 = e$ or $abac = e$. If $(ab)^2 = e$ then $ab = ba$ and G has the following presentation:

$$G = \langle a, b, c \mid a^2 = b^2 = c^2 = e, (ab)^2 = e\rangle.$$

We now compute the abelian invariants of G and G′ as follows:

$$\frac{G}{G'} \cong Z_2 \times Z_2 \times Z_2, \ \ and$$
$$\frac{G'}{G''} \cong Z \times Z \times Z.$$

Therefore, G is infinite, as desired. If $abac = e$ then $aba = c$ and so

$$\begin{aligned} G &= \langle a, b, c \mid a^2 = b^2 = c^2 = e, aba = c\rangle \\ &= \langle a, b \mid a^2 = b^2 = e \rangle \cong Z_2 \blacklozenge Z_2, \end{aligned}$$

Where $Z_2 \blacklozenge Z_2$ denotes the free product of Z_2 by Z_2, which is an infinite group.

Case 2. $a^2 = b^4 = e$ and $c = b^{-1}$. In this case, $b^2 = c^2$ and by existence of a face of length 4, $(ab)^2 = e$ or $aba = b$. If $(ab)^2 = e$ then G has the following presentation:

$$G = \langle a, b \mid a^2 = b^4 = e, (ab)^2 = e \rangle \cong D_8.$$

Therefore, the Cayley graph X on G is isomorphic to the cube Q_3. If $aba = b$ then G has the following presentation:

$$G = \langle a, b \mid a^2 = b^4 = e, ab = ba \rangle \cong Z_2 \times Z_4,$$

and X is isomorphic to Q_3.

Suppose that the 4–faces in X arise only from the relation $b^4=e$. We now consider combinations of generators of length 6. Then $(ab)^3 = e$, or $ab^3ab=e$, or $(ab)^2 = e$ or $(ab^2)^2 = e$. If $ab = ba$ then G is abelian and so it is isomorphic to $Z_2 \times Z_4$ and $X = Cay(G,S) \cong Q_3$. If $(ab)^3 = e$ then G is presented by $\langle a, b \mid a^2 = b^4 = (ab)^3 = e\rangle$. It is well–known that this group is isomorphic to the symmetric group on four symbols, S_4. A simple GAP program [5] shows that the Cayley graph of G is the following ISR (4,6)–fullerene of Figure 2.

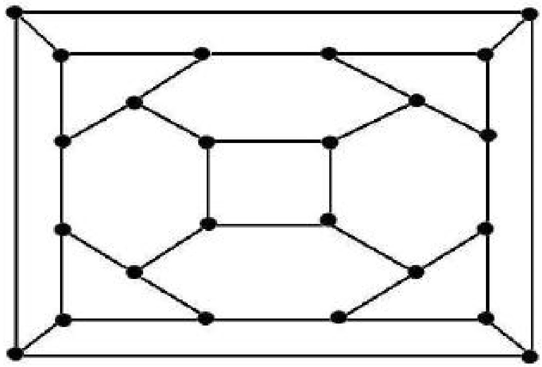

Figure 2. An ISR-Fullerene on 24 vertices.

If $(ab)^2 = e$ then $G = \langle a, b \mid a^2 = b^4 = (ab)^2 = e\rangle \cong D_8$ and $X \cong Q_3$. Finally, if $(ab^2)^2 = e$ then $b^2 \in Z(G)$. Consider the factor group $G/<b^2>$. Then a simple calculation shows that this group can be presented by $\langle a, b \mid a^2 = b^2 = e\rangle \cong Z_2 \blacklozenge Z_2$.

Case 3. $a^2 = b^6 = e$ and $c = b^{-1}$. In this case using a similar argument as those given in Cases 1 and 2, one can see that $(ab)^2 = e$ and so G can be presented as follows:

$$G = \langle a, b \mid a^2 = b^6 = (ab)^2 = e\rangle \cong D_{12},$$

giving the 6–fold prism as its Cayley graph, Figure 3. This completes our argument.

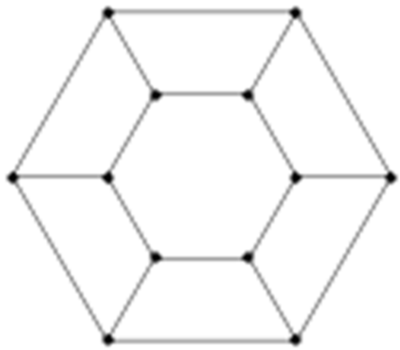

Figure 3. The 6-Prism Graph.

ACKNOWLEDGMENTS

The first author is supported by the University of Kashan under grant no. 364988/36. The research of the second author was in part supported by a grant from Payame Noor Universtiy.

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