Chirality of Toroidal Molecular Graphs

Klavdija Kutnar,† Aleksander Malnič,‡ and Dragan Marušič*,†,‡

University of Primorska, Cankarjeva 5, 6000 Koper, Slovenia, and
Institute of Mathematics, Physics, and Mechanics, Jadranska 19, 1111 Ljubljana, Slovenia

Received May 23, 2005

Symmetry properties of a class of toroidal molecular graphs, arising as covers of certain bipartite cubic Cayley graphs of dihedral groups, are studied. Although these symmetries make all vertices and all edges indistinguishable, they imply intrinsic chirality.

1. INTRODUCTION

The synthesis of spheroidal fullerenes prompted a natural question as to whether similar carbon structures exist on other closed surfaces. As shown in ref 1, such a nonspherical surface can only be the torus, the Klein bottle, or the projective plane. The torus-shaped graphite-like carbon structures—also known as *toroidal graphitoides*, *toroidal polyhexes*, or simply *torusenes*—have received particular attention,[2−14] partly because the other two types are meaningful just from the mathematical viewpoint since they do not admit a realization in the Euclidean 3-space and partly—but more significantly—because torusenes are likely to have direct experimental relevance since "crop circle fullerenes" discovered by Liu[15] in 1997 are presumably torus-shaped.

From a graph-theoretic viewpoint, a torusene is a cubic (trivalent) graph, embedded into the torus in such a way that each face is a hexagon. The description uses three parameters p, q, and t, to be explained below (for theoretic background not defined here, we refer the reader to refs 16, 17, and 18). Formally, a torusene $H(p, q, t)$ is obtained from pq hexagons stacked in an $p \times q$ parallelogram where the two opposite sides are glued together in order to form a tube, and then the top boundary of the tube is glued to the bottom boundary of the tube in order to form a torus. At this last stage, the top part is rotated by t hexagons before the actual gluing takes place. In Figure 1 the $H(8, 1, 2)$ torusene realization of the Moebius−Kantor graph F16 is shown. (Hereafter, the notation FnA, FnB, etc. will refer to the corresponding graphs of order n in the Foster census of all cubic arc-transitive graphs,[19,20] where the symbol FnA is conveniently shortened to Fn whenever such a unique graph exists.) Note that a graph may admit several distinct torusene realizations. For instance, F16 can be realized also as an $H(4, 2, 1)$ torusene.[21]

In chemistry, a molecule is said to be *chiral* if it is not superimposable on its mirror image regardless of how it is contorted. (Similarly, in geometry, a figure is chiral if it has no reflective symmetry, that is, if it is not identical to any of its mirror images.) In particular, a torusene is chiral if no reflection of the torus onto itself preserves the embedded graph. Since biomolecules, such as proteins and enzymes, in living organisms are chiral, therapeutics possessing this property significantly enhance the potential impact of a drug product. Consequently, research involving the concept of chirality appears to be of utmost importance.

Among the spheroidal fullerenes, where the presence of 12 pentagonal faces is needed, only two of them are vertex-transitive and none of them is chiral. These are the buckminsterfullerene C_{60} and the dodecahedron C_{20} (which is nothing but the intersection graph of hexagons of C_{60}). The situation on the torus is completely different since all torusenes are vertex-transitive; moreover, they can be chiral or achiral. For example, the $H(3, 1, 1)$ torusene of the complete bipartite graph $F6 = K_{3,3}$ on six vertices is achiral, while the $H(13, 1, 3)$ torusene of the graph F26 is chiral. A natural question, thus, arises.

Problem 1.1. *For Which Parameters p, q, and t Does There Exist a Chiral Torusene H(p, q, t)?* We note further that many chiral torusenes are, in addition, arc-transitive. It is precisely these torusenes that are the main focus of interest in this article. Hereafter, by a torusene we shall always mean an arc-transitive torusene. In this case, the automorphism group of the underlying cubic graph must contain, by the classical theorem of Tutte,[22] a subgroup G acting regularly on the corresponding set of 1-arcs (arcs in short). In other words, vertex stabilizers of G are isomorphic to $\mathbb{Z}_3$, and therefore, G has no reflections. Such a graph is referred to as *1-regular*, provided this subgroup G coincides with the full automorphism group.

In particular, Problem 1.1 definitely has a positive answer for a triple (p, q, t) whenever there exists a cubic 1-regular graph having an $H(p, q, t)$ torusene realization. Therefore, a partial answer to Problem 1.1 follows from a complete classification of cubic arc-transitive Cayley graphs of dihedral groups.[21] Namely, such a graph is isomorphic either to F6, the cube $F8 = Q_3$, the Heawood graph F14, or the Moebius−Kantor graph F16 or is 1-regular and is isomorphic to a particular graph $\mathscr{D}(n, r)$, where $n \geq 13$ and is odd and $r \in \mathbb{Z}_n^*$ satisfies $r^2 + r + 1 = 0$. (See the subsequent section for its precise description.) Moreover, the graphs $\mathscr{D}(n, r)$ indeed have an $H(n, 1, r)$ torusene realization.

In this article, we make a step forward in regard to Problem 1.1. For an arbitrary graph $\mathscr{D}(n, r)$ and a prime p, coprime with n, we construct a 1-regular $\mathbb{Z}_p^2$ cover of $\mathscr{D}(n, r)$, which is, again, a torusene. (See Section 2 for the definition of a cover.) Its torusene realization must be of the form $H(pn, p, pr)$. The constructions are described in Section 2 and discussed in Section 3. In the Appendix (Section 4), thorough

* Corresponding author e-mail: dragan.marusic@guest.arnes.si.
† University of Primorska.
‡ Institute of Mathematics, Physics, and Mechanics.

10.1021/ci050211t CCC: $30.25
Published on Web 08/26/2005

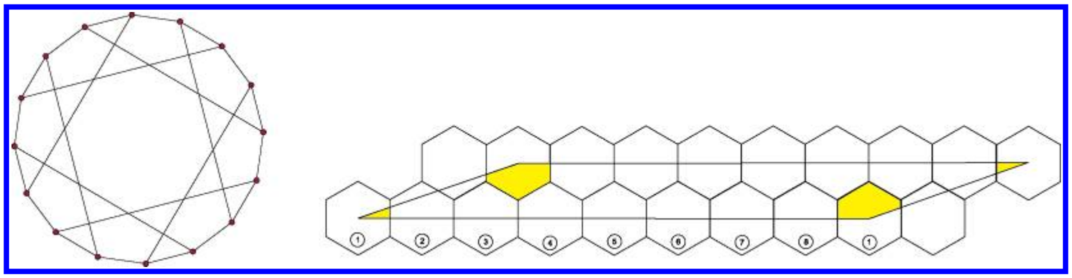

Figure 1. $H(8, 1, 2)$ torusene of the Moebius−Kantor graph F16.

Table 1. 1-Regular Graphs on up to 512 Vertices[a]

		$\mathscr{D}(n, r)$	$\mathscr{CD}(p, n, r)$			$\mathscr{D}(n, r)$	$\mathscr{CD}(p, n, r)$			$\mathscr{D}(n, r)$	$\mathscr{CD}(p, n, r)$
1	F026A	●		29	F218A	●		58	F386A	●	
2	F038A	●		30	*F*222A	●		59	F392A		●
3	F042A	●		31	F224A			60	F398A	●	
4	F056A		●	32	*F*234A		●	61	F400A		
5	F062A	●		33	F248A		●	62	F402A	●	
6	F074A	●		34	F254A	●		63	F416A	●	
7	F078A	●		35	F256D			64	F422A	●	
8	F086A	●		36	F258A	●		65	F432C		
9	F098A	●		37	F266A	●		66	F432E		
10	F104A		●	38	F266B	●		67	F434A	●	
11	F112C			39	F278A	●		68	F434B	●	
12	F114A	●		40	F294B	●		69	F438A	●	
13	F122A	●		41	F296A		●	70	F446A	●	
14	F126A		●	42	F302A	●		71	F448A		
15	F134A	●		43	F304A			72	F448B		
16	F144A			44	F312A		●	73	F456A		●
17	F146A	●		45	F312B			74	F456B		
18	F152A		●	46	F314A	●		75	F458A	●	
19	F158A	●		47	F326A	●		76	F474A	●	
20	F162B			48	F336C			77	F482A	●	
21	F168A		●	49	F336F			78	F488A		●
22	F168E			50	F338A	●		79	F494A	●	
23	F182A	●		51	F342A		●	80	F494B	●	
24	F182B	●		52	F344A		●	81	F496A		
25	A186A	●		53	F350A		●	82	F504A		
26	F194A	●		54	F362A	●		83	F504B		
27	F206A	●		55	F366A	●		84	F504D		
28	F208A			56	F378A			85	F512E		
				57	F378B						

[a] In the first column, each 1-regular graph's name is given as it appears in the Foster census; in the second column, the symbol ● tells us whether it is isomorphic to some $\mathscr{D}(n, r)$, and if it is not, the symbol ● in the third column tells us whether it is isomorphic to some $\mathscr{CD}(p, n, r)$.

and detailed computations are given for the special case of all those elementary abelian covers of the Heawood graph F14 that have a torusene realization.

Let us mention that, according to the revised Foster census,[19,20] there is a total of 406 cubic arc-transitive graphs on up to 512 vertices, of which 85 are 1-regular. Out of these 85 graphs, 46 belong to the class of the above-mentioned graphs $\mathscr{D}(n, r)$. Out of the remaining 39 graphs, an additional 15 can be described via the above-mentioned covering construction (see Table 1). In the computations carried out for the purpose of this article, the use of program package MAGMA[23] has been essential.

Finally, for graph-theoretic and group-theoretic concepts not defined here, we refer the reader to refs 24−27.

2. DESCRIPTION

Recall that the *Cayley graph* of a group G with respect to a inverse-symmetric set of generators $S = S^{-1}$ has vertex set G, with two vertices $g, g' \in G$ being adjacent if and only if $g' = gs$ for some $s \in S$. We are interested here in a particular class of Cayley graphs of dihedral groups arising from a set of generators, all of which are reflections, the so-called cyclic Haar graphs.[28] For an integer n and a subset $S \subseteq \mathbb{Z}_n \backslash \{0\}$, we let $\mathrm{Dih}(n, S)$ denote the Cayley graph of the dihedral group $D_{2n} = \langle a, b | a^n = 1, b^2 = 1, (ab)^2 = 1\rangle$ relative to the generating set $\{ab^s\colon\ s \in S\}$. For the purposes of this article, the vertex set of this graph will be identified with the union of the sets $\{u_i\colon\ i \in \mathbb{Z}_n\}$ and $\{v_i\colon\ i \in \mathbb{Z}_n\}$ and the edge set will consist of all pairs of the form $u_i v_{i+s}$, $s \in S$, $i \in \mathbb{Z}_n$. Further, note that the regular dihedral group is then generated by the permutations ρ and τ mapping according to the respective rules.

$$u_i\rho = u_{i+1},\ v_i\rho = v_{i+1},\quad i \in \mathbb{Z}_n \tag{1}$$

$$u_i\tau = v_{-i},\ v_i\tau = u_{-i},\quad i \in \mathbb{Z}_n \tag{2}$$

For example, the graphs F6, F8, F14, and F16 are isomorphic, respectively, to Dih(3,{0, 1, 2}), Dih(4,{0, 1, 2}), Dih(7,{0, 1, 3}), and Dih(8,{0, 1, 3}).

Now, let $n \geq 7$ be an odd integer such that there exists $r \in \mathbb{Z}_n^*$, satisfying $r^2 + r + 1 = 0$. We shall use a shorthand notation $\mathscr{D}(n, r)$ for the graph $\mathrm{Dih}(n,\{1, r, r^2\})$. (We remark that in ref 21, an equivalent presentation for these graphs was used with the set $\{1, r, r^2\}$, replaced by the set $\{0, 1, r$

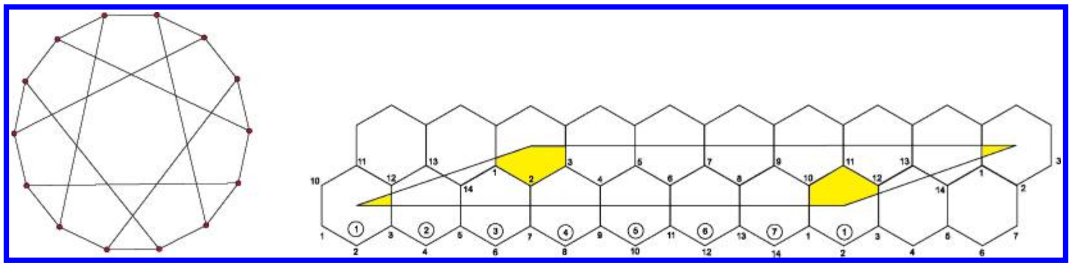

Figure 2. $H(7, 1, 2)$ torusene of the Heawood graph F14.

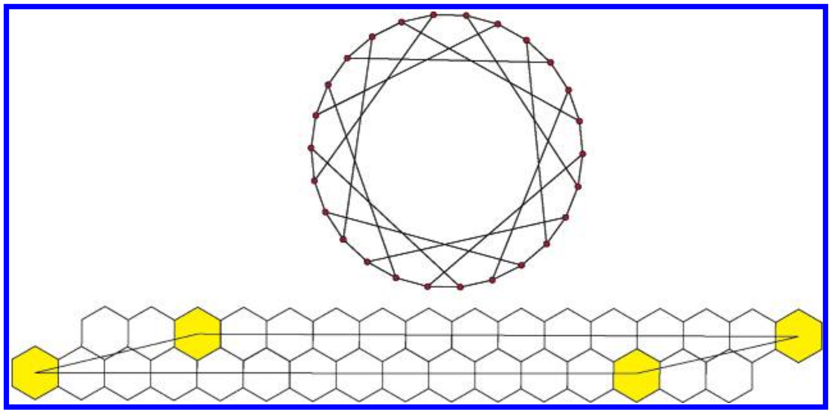

Figure 3. $H(13, 1, 3)$ torusene of F26.

$+ 1\}$. These two presentations give rise to isomorphic graphs because $r - 1$ must be coprime with n.[21]) Note that the permutation σ mapping according to the rule

$$u_i\sigma = u_{ri},\ v_i\sigma = v_{ri}, \quad i \in \mathbb{Z}_n \tag{3}$$

is an automorphism of $\mathscr{D}(n, r)$ such that the group $\langle \rho, \tau, \sigma \rangle$ acts 1-regularly on $\mathscr{D}(n, r)$. As torusenes, these graphs have an $H(n, 1, r)$ realization. In Figure 2, the $H(7, 1, 2)$ torusene realization of F14 is given, and in Figure 3, the $H(13, 1, 3)$ torusene realization of F26 is given.

At this point, we need to recall the concept of graph coverings.[29] Let X be a connected (finite) graph and K a (finite) abelian group. (Note that this last assumption about the group K being abelian is purely technical and is made in order to simplify the discussion later on.) Further, let ζ: $X \to K$ be a *voltage assignment* that associates to each arc (u, v) of X its *voltage* $\zeta(u, v) \in K$ such that $\zeta(u, v) = -\zeta(v, u)$, that is, with inverse arcs carrying inverse voltages. Note that ζ naturally extends to walks by adding the voltages encountered on the arcs of a walk. The *derived regular K-covering graph* Cov(X, ζ) (in short, a *K-cover*) has vertex set $V(X) \times K$ and the adjacency relation defined by $(u, a) \sim (v, a + \zeta(u, v))$, where $u \sim v$ in X and $a \in K$. As a very simple example, note that the cube F8 is a $\mathbb{Z}_2$-cover, the so-called *canonical double cover*, of the tetrahedron graph F4 obtained by assigning the no-identity element in $\mathbb{Z}_2$ to each arc of F4 (See Figure 4). Observe that K acts by left translation onto itself as a group of automorphisms of Cov(X, ζ), called the *group of covering transformations*. Dividing by this action (that is, taking the projection onto the first component) gives rise to a regular K-covering projection $\wp_\zeta$: Cov$(X, \zeta) \to X$. The group of covering transformations is usually denoted by CT$(\wp_\zeta)$. The covering projection (and the derived cover) are called *elementary abelian* whenever K is elementary abelian. For other related concepts, such as lifts of automorphisms, we refer the reader to the Appendix and to refs 30 and 31.

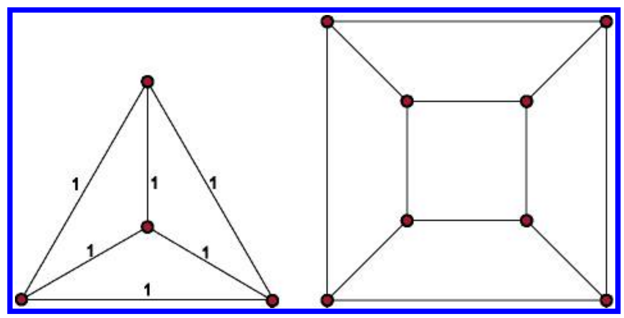

Figure 4. Cube F8 as a canonical double cover of the tetrahedron F4.

We may now define the graphs that arise as regular $\mathbb{Z}_p{}^2$-covers of the graphs $\mathscr{D}(n, r)$. Given a prime p, coprime with n, we let $\mathscr{CD}(p, n, r)$ denote the $\mathbb{Z}_p{}^2$-cover of $\mathscr{D}(n, r)$ arising from the voltage assignment ζ, where

$$\zeta(u_i, v_{i+1}) = e_1 = (1, 0)$$
$$\zeta(u_i, v_{i+\mathrm{r}}) = e_2 = (0, 1)$$
$$\zeta(u_i, v_{i+r^2}) = e_1 + e_2 = (1, 1)$$

for all indices $i \in \mathbb{Z}_n$.

Just like the base graphs $\mathscr{D}(n, r)$, the derived graphs $\mathscr{CD}(p, n, r)$ also have hexagonal embeddings onto the torus, and since they are 1-regular, the corresponding torusenes are chiral and take the form $H(pn, p, pr)$. We give a general discussion of these facts in the next section and a more detailed one for covers of the Heawood graph F14 in the Appendix. In Figures 5−7, a few examples of these embeddings are shown. Let us remark further that in the special case when $n = q$ is a prime and $p = 2$, these graphs may also be constructed as $\mathbb{Z}_q{}^2$-covers of the cube.[32]

To wrap up this section, let us mention another important fact about the graphs $\mathscr{D}(n, r)$, their covers $\mathscr{CD}(p, n, r)$, and the corresponding torusenes. It concerns the concept of the

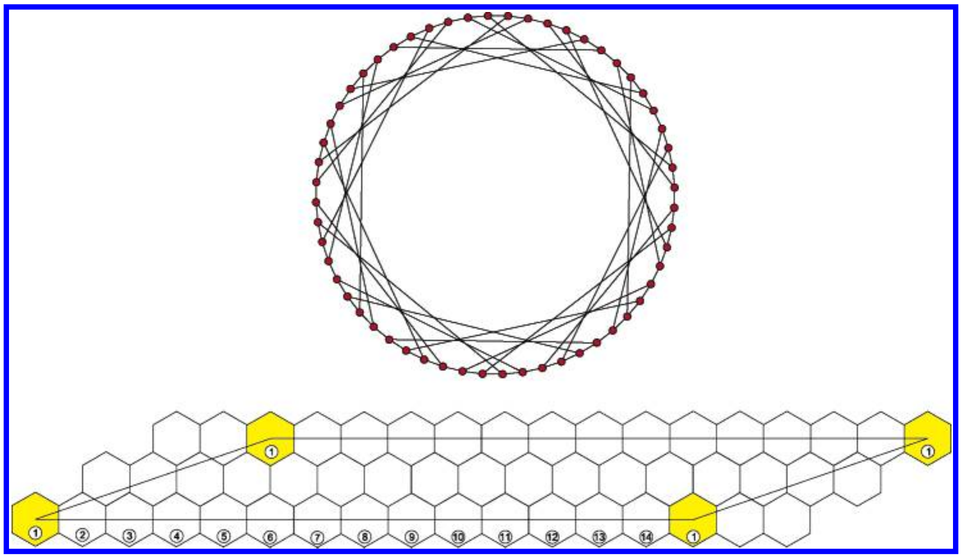

Figure 5. $H(14, 2, 4)$ torusene of F56A, a $\mathbb{Z}_2^2$ cover of F14.

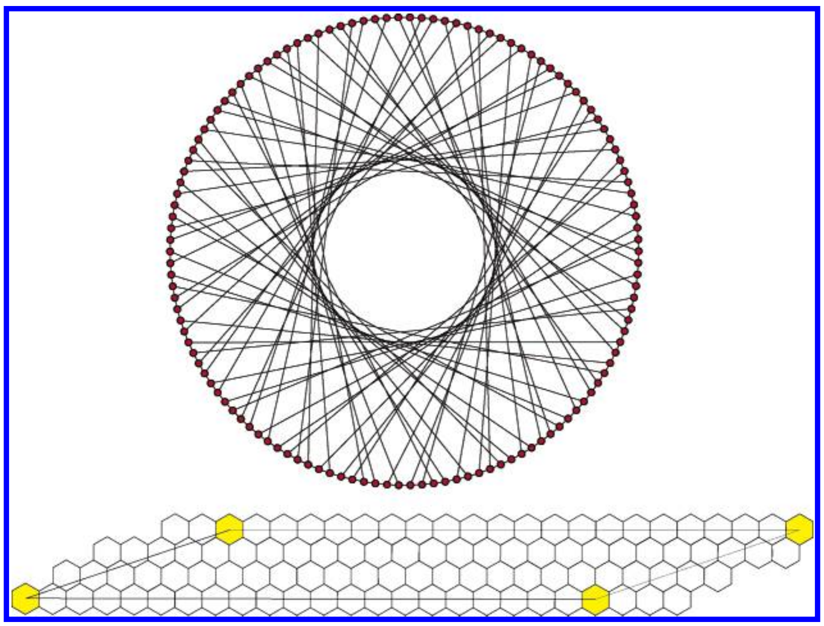

Figure 6. $H(21, 3, 6)$ torusene of F126, a $\mathbb{Z}_3^2$ cover of F14.

so-called consistent cycles. An (oriented) cycle in a graph X is said to be *consistent* if it is rotated by an automorphism of X. It follows by an old unpublished result of Conway that an arc-transitive graph of valency k has $k - 1$ orbits of consistent cycles.[33] Hence, in cubic arc-transitive graphs, there are just two orbits of consistent cycles, and moreover, in a cubic 1-regular graph, there is a "single" orbit of such cycles, if we disregard the cycles orientations. Namely, in a 1-regular cubic graph, two oppositely oriented consistent cycles have the same underlying undirected cycle. In this sense, the consistent cycles in all of our graphs $\mathcal{D}(n, r)$ and $\mathcal{CD}(p, n, r)$ are precisely the hexagonal cells of the toroidal embeddings in question, thus emphasizing the particular symmetry enjoyed by these embeddings.

3. DISCUSSION

We do not discuss here the embeddability of the graphs $\mathcal{CD}(p, n, r)$ onto the torus. In fact, a detailed argument for this is given in the Appendix, and even there only for the smallest base graph, the Heawood graph. However, the arguments in all other cases are analogous. Further, we also leave out the proof that the parameters of these embedding are indeed (pn, p, pr). We do, however, briefly discuss the fact that the graphs $\mathcal{CD}(p, n, r)$ are 1-regular, thus forcing their torus embeddings to be chiral, by outlining the main ideas of the arguments in the proof of this fact.

First, one needs to show that the group $\langle \rho, \tau, \sigma \rangle$ does indeed lift, thus showing that the corresponding $H(pn, p, pr)$ torusenes are arc-transitive. (Again, a detailed proof for the case of the Heawood graph is given in the Appendix.) We may think of the three voltages e_1, e_2, and $e_1 + e_2$ given respectively to all arcs of the forms (u_i, v_{i+1}), (u_i, v_{i+r}), and (u_i, v_{i+r^2}) as colors of the underlying edges. Then, the automorphisms ρ and τ fix the three color classes, whereas the automorphism σ cyclically permutes the three color classes by mapping edges with color class e_1 to those with color class e_2 and so on. On the other hand, ρ and σ preserve the orientation of the arcs, whereas τ reverses this orientation. In view of the known necessary and sufficient conditions for the liftability of automorphisms (an automorphism α lifts

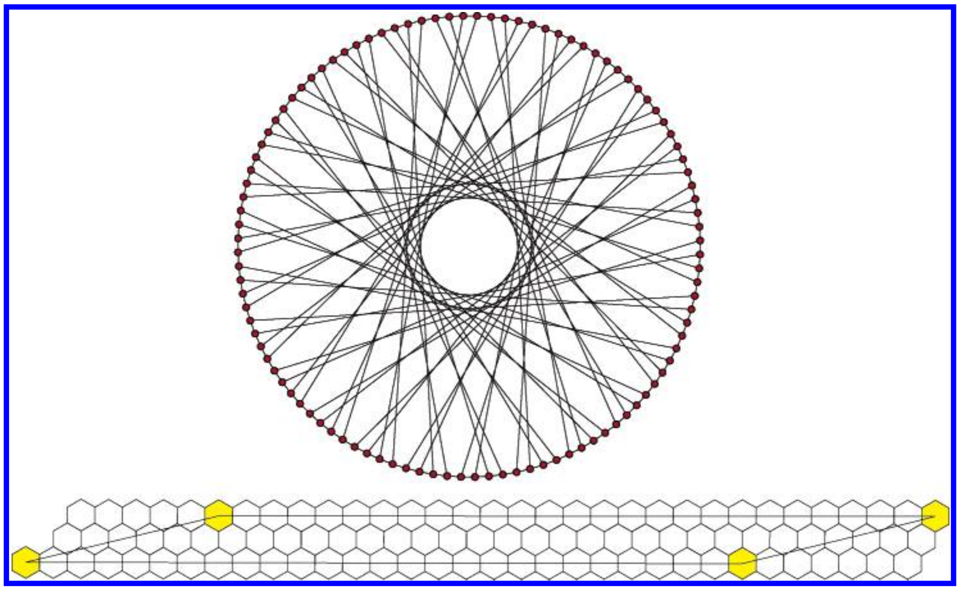

Figure 7. $H(26, 2, 6)$ torusene of F104, a $\mathbb{Z}_2{}^2$ cover of F26.

if and only if the image C^{α} of any cycle C whose voltage is the identity element of the group also has the identity element as its voltage), the proof that both ρ and τ lift is then straightforward, and the proof that σ lifts requires only some minor additional work. (But, see also the Appendix.)

Second, note that the generic 6-cycles in $\mathcal{D}(n, r)$ that give rise to hexagonal cells in the corresponding embeddings $H(n, 1, r)$ are the only 6-cycles in $\mathcal{D}(n, r)$. Furthermore, since their voltages are the identity group element, they give rise to generic six-cycles in $\mathcal{CD}(p, n, r)$, which are, again, the hexagonal cells of the toroidal embeddings. This fact implies, in view of Tutte's result,[22] that the graphs $\mathcal{CD}(p, n, r)$ are either 1-regular or 2-regular. Assuming that a graph $Y = \mathcal{CD}(p, n, r)$ was 2-regular, we would have an involution γ of Y fixing two adjacent vertices and normalizing the lifted group of $\langle \rho, \tau, \sigma \rangle$. But, then t$\gamma$ would clearly have to normalize the group of covering transformations isomorphic to $\mathbb{Z}_p{}^2$ as well, whenever $p \geq 5$, as this group is the Sylow p-subgroup in this case. The cases $p = 2$ and 3 are somewhat more involved, but again, we may see that γ normalizes the group of covering transformations, thus forcing γ to project and contradicting the fact that the base graphs $\mathcal{D}(n, r)$ are only 1-regular. We conclude that the graphs $\mathcal{CD}(p, n, r)$ are indeed 1-regular.

APPENDIX. $\mathbb{Z}_p{}^d$ COVERS OF THE HEAWOOD TORUSENE AND THEIR SYMMETRIES

In this section, we give a detailed analysis of all torusenes arising as elementary abelian covers of the Heawood torusene (such that the respective covering projections of graphs extend to coverings of surfaces). But first, we need to recall some facts about lifting automorphisms.[31]

Let $\wp_{\zeta}$: Cov$(X, \zeta) \rightarrow X$ and $\wp_{\zeta}$: Cov$(X, \zeta') \rightarrow X$ be two covering projections of a connected graph X. We say that $\wp_{\zeta}$ and $\wp_{\zeta'}$ are *isomorphic* if there exists a graph automorphism α of X and an isomorphism $\tilde{\alpha}$: Cov$(X, \zeta) \rightarrow$ Cov(X, ζ') such that $\wp_{\zeta'}\tilde{\alpha} = \alpha\wp_{\zeta}$. Informally, $\tilde{\alpha}$ maps each fiber $\{u\} \times K$ of the first cover bijectively onto the fiber $\{u^{\alpha}\} \times K'$ of the second cover in a manner compatible with the action of α. In particular, if $\wp_{\zeta}$ and $\wp_{\zeta'}$ are isomorphic relative to the identity automorphism $\alpha = $ id, then we say that $\wp_{\zeta}$ and $\wp_{\zeta'}$ are *equivalent*. Note that nonequivalent projections might still be isomorphic. Note further that if we change an existing voltage assignment ζ to ζ' in such a way that $\phi\zeta(C) = \zeta'(C)$ for some automorphism ϕ of K, then the respective projections $\wp_{\zeta}$ and $\wp_{\zeta'}$ are equivalent. In particular, by taking a spanning tree $\mathcal{T}$ of X, one can modify ζ to ζ' so that the arcs in $\mathcal{T}$ receive the trivial voltage and the arcs not in $\mathcal{T}$ receive the ζ-voltage of the respective uniquely defined (oriented) cycle determined by this arc and $\mathcal{T}$. Such a modified assignment is also convenient for deciding whether the derived cover is connected; namely, the voltages of arcs not in $\mathcal{T}$ should generate the group K.

Now suppose that $K = K'$ and $\zeta = \zeta'$ and, hence, $\wp_{\zeta} = \wp_{\zeta'}$. Then, in the above setting, $\tilde{\alpha}$ becomes an automorphism of Cov(X, K), called a *lift* of α along $\wp_{\zeta}$. Observe that if an automorphism has a lift, then it has precisely $|K|$ distinct lifts. For instance, all lifts of the identity automorphism constitute the group of covering transformations CT$(\wp_{\zeta})$. In applications, we want to lift groups of automorphisms, rather than just individual automorphisms. If G is a group of automorphisms of X such that each element of G has a lift along $\wp_K$, then all lifts of all elements of G form a group $\tilde{G}$ of automorphisms of Cov(X, ζ), called the *lift* of G. Observe that if G lifts along $\wp_{\zeta}$, then it lifts along any covering equivalent to $\wp_{\zeta}$, but it might not lift along a covering, isomorphic to $\wp_{\zeta}$ (however, an appropriate conjugate of G does). Clearly, in order for G to lift, it is enough to require that elements from some generating set of G have a lift. Note that the group of covering transformations CT$(\wp_{\zeta})$ is normal in $\tilde{G}$ and that all lifts of an element $\alpha \in G$ constitute precisely a coset of CT$(\wp_{\zeta})$ in $\tilde{G}$ (which implies that $\tilde{G}$/CT$(\wp_{\zeta}) \cong G$). We say that an automorphism of Cov(X, ζ) *projects* along $\wp_{\zeta}$ if it is fiber-preserving, that is, if it arises as a lift of some automorphism of X. This happens if and only if such an automorphism normalizes CT$(\wp_{\zeta})$. Thus, if CT$(\wp_{\zeta})$ is not normal in Cov(X, ζ), then the derived graph has symmetries that do not arise as lifts of symmetries of X, and studying these is much harder.

As a last remark, observe that when considering embedded graphs, we normally take into account only those automorphisms of the graph that extend to automorphisms of the

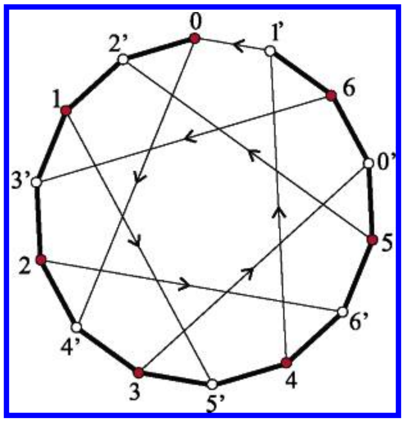

Figure 8. Heawood graph F14.

surface. This means that graph covers arising from non-equivalent or nonisomorphic covering projections as embedded graphs can still be isomorphic or even equivalent as abstract graphs. In what follows, we address these questions only in the limited context of surface automorphisms and those covering projections of graphs that extend to coverings of the supporting surfaces.

Coming back to torusenes arising as elementary abelian covers of the Heawood torusene, it transpires that such covers are either cyclic $\mathbb{Z}_p$ -covers or $\mathbb{Z}_p{}^2$-covers. As for the latter, for each prime p, such a unique (up to equivalence of projections) covering exists, and as we shall see, the full surface automorphism group lifts. If $p \neq 7$, the respective voltage assignments can be chosen in a nice "symmetric" way, showing that the graphs coincide with the covers $\mathcal{CD}(p, 7, 2)$ defined in Section 2. In contrast with this, the prime cyclic covers behave differently. For one thing, $p + 1$ pairwise non-equivalent $\mathbb{Z}_p$-covering projections exist, some of which might even be pairwise nonisomorphic. In addition, the maximal group that lifts need not be the full surface automorphism group. This depends on the congruence class of p modulo 3. In certain cases, the derived embeddings are chiral.

Let $\mathcal{H}$ denote the Heawood graph (we shall use this shorter notation instead of Foster Census notation F14). With notation as in Figure 8, choose the *principal* (oriented) Hamiltonian cycle to be

$$C_H = (0, 2', 1, 3', 2, 4', 3, 5', 4, 6', 5, 0', 6, 1', 0)$$

and let $\mathcal{T}$ denote the spanning tree formed by the edges of $C_H\backslash 1'0$. Next, denote by C_j ($j \in \mathbb{Z}_7$) the (oriented) cycles determined by $\mathcal{T}$ and the seven chordal arcs $04'$, $15'$, $26'$, $30'$, $41'$, $52'$, $63'$, and $1'0$, respectively. Then

$$C_0, C_1, C_2, C_3, C_4, C_5, C_6, C_H$$

is an (ordered) basis of the first homology group H_1 ($\mathcal{H}$; $\mathbb{Z}_p$), viewed as the vector space over the prime field $\mathbb{Z}_p$. Let ζ: $\mathcal{H} \to \mathbb{Z}_p{}^d$ be a voltage assignment on the arcs of $\mathcal{H}$ where we may, without loss of generality, assume that the arcs on $\mathcal{T}$ carry the trivial voltage. Let z_j ($j \in \mathbb{Z}_7$) and z_H denote the (so-far unknown) voltages of the arcs $04'$, $15'$, $26'$, $30'$, $41'$, $52'$, $63'$, and $1'0$, respectively. Extending the voltage assignments to walks, we have that

$$\zeta(C_j) = z_j \ (j \in \mathbb{Z}_7) \text{ and } \zeta(C_H) = z_H$$

Table 2. The Voltages on Faces

$\zeta(C_{F_0})$	$\zeta(C_{F_1})$	$\zeta(C_{F_2})$	$\zeta(C_{F_3})$	$\zeta(C_{F_4})$	$\zeta(C_{F_5})$	$\zeta(C_{F_6})$
$z_0 - z_1$	$z_1 - z_2$	$z_2 - z_3$	$z_3 - z_4$	$z_4 - z_5 + z_H$	$z_5 - z_6$	$z_6 - z_0 - z_H$

We now find the unknown voltages so that the derived covering graph embeds into the torus (and the respective covering projection extends to a covering of surfaces). It is generally known[29] that the characteristic $\tilde{\chi}$ of such a derived embedding is given by the Riemann−Hurwitz formula

$$\tilde{\chi} = n\chi - n \sum_F (1 - 1/r_F)$$

where χ is the characteristic of the base embedding, n is the size of the voltage group, and for each face F, the order of the voltage $\zeta(F)$ associated with its boundary cycle is denoted by r_F. In our case, we have $\chi = 0$. So, $\tilde{\chi} = 0$ if and only if $\sum_F(1 - 1/r_F) = 0$; that is, for each face, one has $r_F = 1$ (as expected since the covering of surfaces must be unbranched). This is equivalent to saying that the voltage of the boundary cycle of each face is trivial. In particular, recall that the (genus) embedding $H(7, 1, 2)$ of $\mathcal{H}$ into the torus, see Figure 2, has seven hexagonal faces bounded by the following cycles $F_0 = C_0 - C_1$, $F_1 = C_1 - C_2$, $F_2 = C_2 - C_3$, $F_3 = C_3 - C_4$, $F_4 = C_4 - C_5 + C_H$, $F_5 = C_5 - C_6$, and $F_6 = C_6 - C_0 - C_H$. (Observe that this is just one possibility for choosing which of the 6-cycles in $\mathcal{H}$ are facial. However, a different choice leads to an isomorphic embedding; hence, we may, without loss of generality, restrict ourselves to the particular embedding above.) The respective voltages are given in Table 2. Consequently, the derived covering embedding of the Heawood torusene above is, again, a torusene if and only if

$$z_4 = z_3 = z_2 = z_1 = z_0 = a,\ z_5 = z_6 = a + b, \text{ and } z_H = b \tag{4}$$

for some a, $b \in \mathbb{Z}_p{}^d$. Since the covering is assumed to be connected, the voltages assigned to the base homology cycles must generate the whole voltage group, that is, $\langle a, b, a + b\rangle = \langle a, b\rangle = \mathbb{Z}_p{}^d$. Thus, $d = 1$ or $d = 2$.

Before sorting out all pairwise nonequivalent (or possibly nonisomorphic) coverings in each of the two cases above, and in order to discuss their symmetries, a few words about the automorphism group of $\mathcal{H}$ are in order. Consider the following elements of Aut$\mathcal{H}$:

$$\rho = (0, 1, 2, 3, 4, 5, 6)(0', 1', 2', 3', 4', 5', 6')$$
$$\sigma = (0)(1, 2, 4)(3, 6, 5)(0')(1', 2', 4')(3', 6', 5')$$
$$\tau = (0, 0')(1, 6')(2, 5')(3, 4')(4, 3')(5, 2')(6, 1')$$
$$\omega = (1, 5)(4, 6)(0', 5')(3', 6')(0)(2)(3)(1')(2')(4')$$

The group

$$\Gamma_{14} = \langle \rho, \tau\rangle \cong D_7$$

is vertex-transitive on $\mathcal{H}$. In fact, it is a minimal vertex-transitive subgroup since it acts regularly on the vertex set of $\mathcal{H}$, showing that the Heawood graph is a Cayley graph of the group $\langle \rho, \tau\rangle$ with respect to the generating set of involutions $\{\rho\tau, \rho^2\tau, \rho^4\tau\}$. The group

$$\Gamma_{21} = \langle \rho, \sigma\rangle \cong \mathbb{Z}_7 : \mathbb{Z}_3$$

is edge- but not vertex-transitive, acting regularly on the set of edges (and, hence, minimal among groups preserving the two set of the bipartition of $\mathscr{H}$). The group

$$\Gamma_{42} = \langle \rho, \sigma, \tau \rangle \cong \mathbb{Z}_7 : \mathbb{Z}_6$$

is arc-transitive on $\mathscr{H}$, acting regularly on the set of arcs, and, hence, a minimal such subgroup of Aut$\mathscr{H}$. [Observe that Γ_{42} is the full automorphism group Aut$H(7, 1, 2)$ of the toroidal embedding of $\mathscr{H}$. Note, however, that Aut$\mathscr{H}$ contains subgroups, conjugate to Γ_{14}, Γ_{21}, and Γ_{42}. Which copy of Γ_{42} will figure as the automorphism group of the embedding depends on the actual choice of faces.] Obviously, Γ_{14} and Γ_{21} are maximal in Γ_{42}. Moreover, Γ_{42} is maximal in the full automorphism group Aut$\mathscr{H} = \langle \rho, \omega, \tau \rangle \cong$ PGL(2, 7) of order 336. Finally, let us mention that Aut$_0\mathscr{H} = \langle \rho, \omega \rangle \cong$ PSL(2, 7) $\cong$ GL(3, 2) is the unique largest subgroup preserving the two sets of the bipartition of $\mathscr{H}$ and is, hence, of index 2 in Aut$\mathscr{H}$.

Case $K = \mathbb{Z}_p^2$. In this case, a and b, as in eq 4, must be linearly independent as vectors over $\mathbb{Z}_p$. Recall that changing the voltage assignments by an arbitrary automorphism of K preserves the equivalence class of covering projections, and note that, since the faces of the base embedding carry the trivial voltage, we also do not change the equivalence class of surface coverings. Therefore, since Aut$\mathbb{Z}_p^2 \cong$ GL(2, p) acts transitively on the set of bases of $\mathbb{Z}_p^2$, we can, without loss of generality, assume that

$$a = (1, 0) \text{ and } b = (0, 1)$$

Moreover, if $p \neq 7$, we can find a more "symmetric" assignment so that the voltages of arcs on the principal Hamiltonian cycle (relative to the chosen orientation of C_H) alternate between two values and the chordal arcs (also relative to the orientation of C_H) carry the same voltage, thus making the graph isomorphic to our graph $\mathscr{CD}(p, 7, 2)$. By computation, we get

$$\zeta(j, (j+2)') = (1, 0),\ \zeta(j', j-1) = (0, 1),\ \zeta(j, (j+4)') = (1, 1),\ (j \in \mathbb{Z}_7)$$

If $p = 7$, finding such a "symmetric" assignment is impossible since the principal Hamiltonian cycle C_H would then have trivial voltage.

Let us now discuss the symmetries of the derived covering torusene, namely, those that arise as lifts of surface automorphisms of the embedding of $\mathscr{H}$. We first recall the basic lifting lemma,[30,31] which has already been mentioned in Section 3. This lemma can also be stated as follows: a graph automorphism ϕ lifts along a regular covering projection, where the voltage group is abelian, if and only if the mapping of voltages

$$\phi^{\#}\colon\ \zeta(C) \rightarrow \zeta(C^{\phi})$$

where C ranges over the base homology cycles, extends to an automorphism of the voltage group. Since we are mainly interested in group Γ_{42}, let us, therefore, consider the action of its generators ρ, τ, and σ on the base homology cycles. In the computation below, we always assume that the assignment is the general "asymmetrical" one, with the arcs of $\mathscr{T}$ carrying the trivial voltage.

Table 3. The Action of the Generators of Aut$H(7, 1, 2)$ on the Base Homology Cycles

	ρ	τ	σ
C_0	C_1	$-C_3$	$-C_0 - C_2 - C_4 - C_H$
C_1	C_2	$-C_2$	$-C_2 - C_4 - C_6$
C_2	C_3	$-C_1$	$-C_1 - C_4 - C_6$
C_3	C_4	$-C_0$	$-C_1 - C_3 - C_6$
C_4	$C_5 - C_H$	$-C_6 + C_H$	$-C_1 - C_3 - C_5$
C_5	C_6	$-C_5$	$C_1 + C_2 + C_4 + C_6$
C_6	$C_0 + C_H$	$-C_4 - C_H$	$C_1 + C_3 + C_4 + C_6$
C_H	C_H	$-C_H$	$\sum_{j=0}^{6} C_j$

From Table 3, it follows that $\rho^{\#}$: $a \rightarrow a$ and $\rho^{\#}$: $b \rightarrow b$. This clearly extends to the identity automorphism. Hence, ρ lifts. Next, $\tau^{\#}$: $a \rightarrow -a$ and $\tau^{\#}$: $b \rightarrow -b$. As the voltage group is abelian, multiplication by -1 (that is, taking the additive inverse) extends to an automorphism of $\mathbb{Z}_p^2$. Hence, τ lifts. As for the automorphism σ, we have that $\sigma^{\#}$: $a \rightarrow -3a - b$ and $\sigma^{\#}$: $b \rightarrow 7a + 2b$. Since the matrix

$$\begin{pmatrix} -3 & 7 \\ -1 & 2 \end{pmatrix}$$

is invertible over $\mathbb{Z}_p$, the mapping $\sigma^{\#}$ extends to an automorphism. Thus, σ lifts.

We conclude that the full surface automorphism group Γ_{42} lifts to a group of automorphisms of the derived covering embedding. Although we are mainly interested in surface automorphisms, one can easily see that Γ_{42} is actually the maximal group that lifts along the respective projection of graphs. Namely, recall that Γ_{42} is a maximal subgroup of Aut$\mathscr{H}$, and observe that the graph automorphism ω does not lift. (One can check, for instance, that $\omega(C_1) = -C_3 + C_2$. So, $\omega^{\#}$: $a \rightarrow 0$, and hence, $\omega^{\#}$ cannot extend to an automorphism of $\mathbb{Z}_p^2$ since $a \neq 0$, as required.)

These observations imply that the derived covering torusenes are chiral. If p is equal to 2, 3, 5, or 7, then the derived graphs have orders 56, 126, 350, and 686, respectively. By Conder and Dobcsanyi's list,[20] all arc-transitive graphs with these orders and a girth of 6 are exactly 1-transitive. Therefore, the full automorphism group of our torusenes must be $\tilde{\Gamma}_{42}$. Let $p > 7$, and suppose that the derived torusene is reflexible. Then, $\tilde{\Gamma}_{42}$ is of index 2 in the full automorphism group of the embedding. As $\mathbb{Z}_p^2$ is now characteristic in $\tilde{\Gamma}_{42}$, it is normal in the larger group, which must then project, which is a contradiction. This shows that the derived coverings are indeed chiral. Furthermore, the parameters of the respective chiral torusenes are $(7p, p, 2p)$.

Case $K = \mathbb{Z}_p$. The vector $[\zeta(C_0), \zeta(C_1), \zeta(C_2), \zeta(C_3), \zeta(C_4), \zeta(C_5), \zeta(C_6), \zeta(C_H)]^t$ of voltage assignments can be written, in view of eq 4 and the fact that, now, $a, b \in \mathbb{Z}_p$, as

$$a(1, 1, 1, 1, 1, 1, 1, 0)^t + b(0, 0, 0, 0, 0, 1, 1, 1)^t$$

The action of Aut$\mathbb{Z}_p$, that is, multiplication by a nonzero element of $\mathbb{Z}_p$, leaves invariant any one-dimensional subspace generated by such a vector of voltage assignments. Thus, the number of pairwise nonequivalent covering projections is equal to the number of one-dimensional subspaces contained in the two-dimensional subspace $U = \langle (1, 1, 1, 1, 1, 1, 1, 0)^t, (0, 0, 0, 0, 0, 1, 1, 1)^t \rangle$ of $\mathbb{Z}_p^8$. There are $p + 1$ such subspaces, conveniently parametrized as

$$U(s) = \langle s(1, 1, 1, 1, 1, 1, 1, 0)^t + (0, 0, 0, 0, 0, 1, 1, 1)^t\rangle \quad (s \in \mathbb{Z}_p),\ U(\infty) = \langle(1, 1, 1, 1, 1, 1, 1, 0)^t\rangle$$

Note that the above pairwise nonequivalent covering projections might not all be pairwise nonisomorphic. That is, there might exist surface isomorphisms taking one covering to another, which "project" to automorphisms of the Heawood torusene.

So, let us consider the question, which surface automorphisms lift? As before, we have, from Table 3, that $\rho^\#$ extends to the identity automorphism and $\tau^\#$ corresponds to multiplication by -1. Thus, the dihedral group Γ_{14} lifts. However, the answer as to whether σ lifts depends on the congruence class of the prime p modulo 3. Namely, recall that $\sigma^\#$ maps according to the rules $\sigma^\#$: $a \rightarrow -3a - b$ and $\sigma^\#$: $b \rightarrow 7a + 2b$. In order for $\sigma^\#$ to extend to an automorphism of $\mathbb{Z}_p$, there must exist $\lambda \in \mathbb{Z}_p^*$ such that $\sigma^\#(x) = \lambda x$. That is, $(a, b)^t$ is a λ eigenvector for the matrix

$$\begin{pmatrix} -3 & -1 \\ 7 & 2 \end{pmatrix} \tag{5}$$

Observe that the above matrix represents the action of $\sigma^\#$ on the two-dimensional subspace U of $\mathbb{Z}_p^8$, expressed in the (ordered) basis of column vectors $(1, 1, 1, 1, 1, 1, 1, 0)^t$ and $(0, 0, 0, 0, 0, 1, 1, 1)^t$. Note that U is indeed invariant under this action since σ lifts in the case $K = \mathbb{Z}_p^2$. Now, the characteristic polynomial of the above matrix is $\kappa(x) = x^2 + x + 1$. There are three subcases to consider.

Subcase $p \equiv -1$ (mod 3). In this case, $\kappa(\lambda)$ has no roots in $\mathbb{Z}_p$. Hence, σ does not lift. Consequently, Γ_{14} is the largest (surface) group that lifts, in view of the fact that it is maximal in Γ_{42}. Note further that since σ is of order 3 and the matrix (eq 5) has no invariant subspaces on U, there are $(p + 1)/3$ orbits of one-dimensional subspaces of U. The embeddings arising from voltage assignments in the same orbit are isomorphic as surface coverings and nonisomorphic if arising from different orbits. We omit the discussion whether these embeddings are isomorphic (not as coverings), and we address neither the question as to what is their actual surface automorphism group nor that regarding their chirality.

Subcase $p \equiv 1$ (mod 3). In this case, the characteristic polynomial $\kappa(\lambda)$ has two distinct roots $\lambda_j \in \mathbb{Z}_p$ ($j = 1, 2$), each with a corresponding eigenvector $(1, -\lambda_j - 3)^t$. (Note: computations are also valid in the case of $p = 7$, where $\lambda_1 = -3$ and $\lambda_2 = 2$.) The two covering projections arising from the vector of voltage assignments

$$(1, 1, 1, 1, 1, -\lambda_j - 2, -\lambda_j - 2, -\lambda_j - 3)^t, (j = 1, 2)$$

are nonisomorphic (as surface coverings), and the whole surface automorphism group Γ_{42} lifts. Actually, Γ_{42} is, in fact, the largest group that lifts along the respective projection of graphs, for one can check that ω does not lift. This helps to settle the question about the chirality of the derived torusenes. Namely, let $p > 7$ and suppose that the embedding is reflexible. Then, $\tilde{\Gamma}_{42}$ is of index 2 in the full automorphism group of the embedding. As $\mathbb{Z}_p$ is now characteristic in $\tilde{\Gamma}_{42}$, it is normal in the larger group, which must then project, which is a contradiction. Hence, the embeddings are chiral. If $p = 7$, then one gets two arc-transitive graphs on 98 vertices, one arising from the voltage assignment $(1, 1, 1, 1, 1, 1, 1, 0)^t$ and the other from $(1, 1, 1, 1, 1, 0, 0, -1)^t$. By Conder and Dobcsanyi's list,[20] one of these is 1-regular, and hence chiral, and the other 2-regular, and hence reflexible. Explicit checking reveals that the one arising from $(1, 1, 1, 1, 1, 0, 0, -1)^t$ is chiral.

The remaining one-dimensional subspaces fall into $(p - 1)/3$ distinct orbits, giving rise to pairwise nonisomorphic coverings. Group Γ_{14} is the maximal one that lifts. We again omit further discussion of these derived embeddings.

Subcase $p = 3$. In this case, $\kappa(\lambda)$ has a unique root $\lambda = 1$, and the respective eigenspace is spanned by $(a, b)^t = (1, -1)^t$. There are two orbits of $\sigma^\#$ acting on the one-dimensional subspaces of U. The one spanned by $(1, 1, 1, 1, 1, 0, 0, -1)^t$ gives rise to the derived covering embedding with the property that Γ_{42} lifts. By Conder and Dobcsanyi's list,[20] the obtained graph is indeed 1-regular, and hence, the embedding is chiral. The other three subspaces give rise to coverings, isomorphic to the one arising from the voltage assignment $(1, 1, 1, 1, 1, 1, 1, 0)^t$. The maximal group that lifts is the dihedral group Γ_{14}. The derived graph is vertex-transitive but not arc-transitive since there is a unique arc-transitive graph on 42 vertices, namely, the one arising from $(1, 1, 1, 1, 1, 0, 0, -1)^t$. We leave out the discussion of its chirality.

ACKNOWLEDGMENT

Supported, in part, by Ministrstvo za visoko šolstvo, znanost in tehnologijo Slovenije, Program No. P1-0285 (K.K. and D.M.) and Program No. P1-0285 (A.M. and D.M.).

Note Added after ASAP Publication. This article was released ASAP on August 26, 2005 with the graphics of Figures 1 and 2 transposed. The correct version was posted on November 16, 2005.

REFERENCES AND NOTES

(1) Deza, M.; Fowler, P. W.; Rossat, A.; Rogers, K. M. Fullerenes as tilings of surfaces. *J. Chem. Inf. Comput. Sci.* **2000**, *9*, 550−558.
(2) Diudea, M. V.; Kirby, E. C. The energetic stability of tori and single-wall tubes. *Fullerene Sci. Technol.* **2001**, *9*, 445−465.
(3) Diudea, M. V.; Silaghi-Dumitrescu, I.; Parv, B. Toranes versus torenes. *MATCH* **2001**, *44*, 117−133.
(4) Diudea, M. V. Topology of naphthylenic tori. *Phys. Chem. Chem. Phys.* **2002**, *19*, 4740−4746.
(5) Diudea, M. V. Toroidal graphenes from 4-valent tori. *Bull. Chem. Soc. Jpn.* **2002**, *75*, 487−492.
(6) Diudea, M. V.; John, P. E.; Graovac, A.; Primorac, M.; Pisanski, T. Leapfrog and related operations on toroidal fullerenes. *Croat. Chem. Acta* **2003**, *76*, 153−159.
(7) Diudea, M. V.; Parv, B.; Kirby, E. C. Azulenic tori. *MATCH* **2003**, *47*, 53−70.
(8) Diudea, M. V.; Janežič, D.; Graovac, A. Topology counting in nanostructures. *Carpath. J. Math.* **2004**, *20*, 223−234.
(9) Kirby, E. C.; Mallion, R. B.; Pollak, P. Toroidal polyhexes. *J. Chem. Soc., Faraday Trans.* **1993**, *89*, 1945−1953.
(10) Graovac, A.; Plavšič, D.; Kaufman, M.; Kirby, E. C.; Pisanski, T. Application of the adjacency matrix eigenvectors method to geometry determination of toroidal carbon molecules. *J. Chem. Phys.* **2000**, *113*, 1925−1931.
(11) John, P. E.; Kekulé count in toroidal hexagonal carbon cages. *Croat. Chem. Acta* **1998**, *71*, 435−447.
(12) Kirby, E. C.; Pollak, P. How to enumerate the connectional isomers of a toroidal polyhex fullerene. *J. Chem. Inf. Comput. Sci.* **1998**, *38*, 66−70.
(13) Lijnen, E.; Ceulemans, A. Oriented 2-cell embeddings of a graph and their symmetry classification: generating algorithms and case study of the Moebius−Kantor graph. *J. Chem. Inf. Comput. Sci.* **2004**, *44*, 1552−1564.

(14) Xiao, J. Y.; Hosoya, H. Analysis of the relationship among the graphs isomorphic to multilayered cyclic fence graphs (MLCFG). *J. Chem. Inf. Comput. Sci.* **2002**, *42*, 1004−1010.
(15) Liu, J.; Dai, H. J.; Hafner, J. H.; Colbert, D. T.; Smalley, D. T. R. E.; Tans, S. T.; Dekker, C. Fullerene crop circles. *Nature* **1997**, *385*, 780−781.
(16) Altshuler, A. Hamiltonian circuits in some maps on the torus. *Discrete Math.* **1972**, *1*, 299−314.
(17) Altshuler, A. Construction and enumeration of regular maps on the torus. *Discrete Math.* **1973**, *4*, 201−217.
(18) Thomassen, C. Tilings of the torus and the Klein bottle and vertex-transitive graphs on a fixed surface. *Trans. Am. Math. Soc.* **1991**, *323*, 605−635.
(19) *The Foster Census*; Bouwer, I. Z., Ed.; Charles Babbage Research Centre: Winnipeg, Canada, 1988.
(20) Conder, M. D. E.; Dobcsanyi, P. Trivalent symmetric graphs on up to 768 vertices. *J. Comb. Math. Comb. Comput.* **2002**, *40*, 41−63.
(21) Marušič, D.; Pisanski, T. Symmetries of hexagonal molecular graphs on the torus. *Croat. Chem. Acta* **2000**, *73*, 969−981.
(22) Tutte, W. T. A family of cubical graphs. *Proc. Cambridge Philos. Soc.* **1947**, *43*, 459−474.
(23) Bosma, W.; Cannon, J.; Playoust, C. The MAGMA Algebra System I: The User Language. *J. Symbolic Comput.* **1997**, *24*, 235−265.
(24) Biggs, N. L.; White, A. T. *Permutation groups and combinatorial structures*; Cambridge University Press: New York, 1979.
(25) Bondy, A.; Murty, U. S. R. *Graph Theory with Applications*; American Elsevier Co.: New York, 1976.
(26) Coxeter, H. S. M.; Moser, W. O. J. *Generators and Relators for Discrete Groups*, 4th ed.; Springer-Verlag: New York, 1980.
(27) Wielandt, H. *Finite Permutation Groups*; Academic Press: New York, 1964.
(28) Hladnik, M.; Marušič, D.; Pisanski, T. Cyclic Haar graphs. *Discrete Math.* **2002**, *244*, 137−152.
(29) Gross, J. L.; Tucker, T. W. *Topological Graph Theory*; Wiley Interscience: New York, 1987.
(30) Malnič, A.; Nedela, R.; Škoviera, M. Lifting graph automorphisms by voltage assignments. *Eur. J. Combin.* **2000**, *21*, 927−947.
(31) Malnič, A.; Marušič, D.; Potočnik, P. Elementary abelian covers of graphs. *J. Algebr. Comb.* **2004**, *20*, 71−97.
(32) Feng, Y. Q.; Kwak, J. H.; Wang, K. S. Classifying cubic symmetric graphs of order $8p$ or $8p^2$. *Eur. J. Combin.* **2005**, in print.
(33) Biggs, N. L. Aspects of symmetry in graphs, Algebraic methods in graph theory. *Colloq. Math. Soc. Janos Bolyai*; North-Holland: Amsterdam−New York, 1981; Vols. I and II (Szeged, 1978), pp 27−35.

CI050211T