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Symmetries of Hexagonal Molecular Graphs on the Torus

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Symmetric properties of some molecular graphs on the torus are studied. In particular we determine which cubic cyclic Haar graphs are 1-regular, which is equivalent to saying that their line graphs are ½-arc-transitive. Although these symmetries make all vertices and all edges indistinguishable, they imply intrinsic chirality of the corresponding molecular graph.

Key words: molecular graphs, hexagonal molecular graphs.

INTRODUCTORY REMARKS

Following the discovery and synthesis of spheroidal fullerenes, a natural question arises as to whether there exist torus-shaped graphite-like carbon structures which were given different names such as toroidal graphitoides or torusenes (see for instance Refs. 1–5). Indeed, they have been recently experimentally detected (see Ref. 4). Their graphs are cubic (trivalent), embedded onto torus. The geometry of these objects might afford new opportunities for holding reacting substrates in position. Unlike ordinary fullerenes that need the presence of twelve pentagonal faces, torusenes can be completely tessellated by hexagons.

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Buckminsterfullerene C_{60}, which is the most abundant fullerene, exhibits a high degree of symmetry. In particular, it is together with the dodecahedron C_{20}, the only vertex-transitive fullerene. The situation on the torus is quite different since there every hexagonal tessellation is vertex-transitive. On the other hand, the buckminsterfullerene is known to be achiral, while torus allows for highly symmetric chiral torusenes. Each hexagonal tessellation on the torus gives rise (*via* the line graph-medial graph construction) to a tetravalent net composed of triangles, where each triangle corresponds to a vertex in the original tessellation and is joined with three other triangles, with the remaining faces being hexagons corresponding to the hexagons in the original tessellation (see Figure 1).

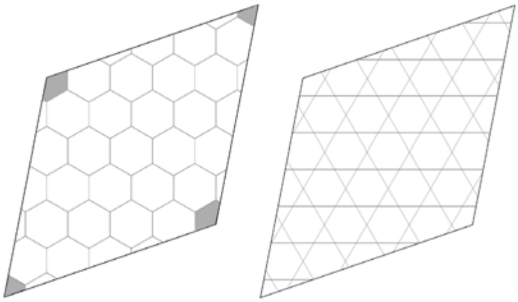

Figure 1. A hexagonal trivalent tessellation and its tetravalent line graph.

In general, the symmetry of a graph may be higher than the symmetry of the underlying carbon cage (combinatorial map). Such is the situation, for example, with the so-called Heawood graph of order 14, that is, the Levi graph (see Ref. 6) of the Fano configuration, which in addition to automorphisms preserving hexagonal face structure (42 in all), allows additional automorphisms (a total of 336); see Figure 2.

In this paper we restrict our attention to a class of cubic graphs embedded on the torus with the property that all of the faces are hexagons. From now on by a torusene we shall mean such an embedded graph. It transpires that each torusene can be described by three parameters p, q, and t, explained hereafter (for theoretical background, see Refs. 7–9). A torusene $H(p, q, t)$ is obtained from $p \times q$ hexagons stacked in a $p \times q$-parallelogram where the two 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 so as to form a torus. In this last stage the top part is rotated by t hexagons before the actual gluing is taking place. (See Figure 3 for an example.) The algorithm that identifies isomorphic torusenes and finds, for each isomorphism

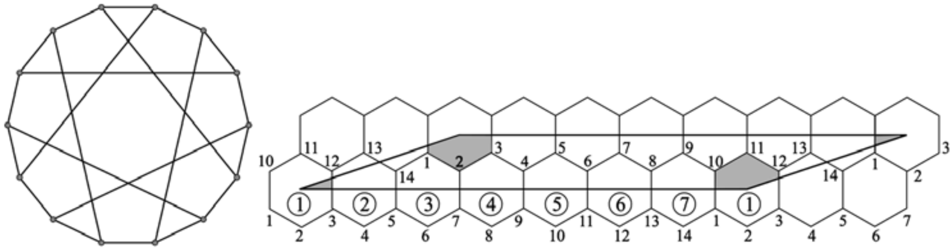

Figure 2. The Heawood graph is the Levi graph of the Fano configuration. It has 14 vertices. Its embedding on torus H(7,1,2) has 7 hexagons. There are 42 automorphisms preserving the embedding out of a total of 336 automorphisms.

class, the canonical parameters (p, q, t) is given in Ref. 3. However, note that our notation $\mathrm{H}(p, q, t)$ corresponds to $\mathrm{TPH}(a, b, d)$ of Refs. 2 and 3, where $p = a$, $q = d$, $t = b-d$.

It transpires that all graphs $\mathrm{H}(p, q, t)$ possess a high degree of symmetry. They are all vertex-transitive. In this paper we are concerned with the problem of determining which graphs $X = \mathrm{H}(p, q, t)$ are 1-regular? This means that the automorphism group Aut X acts transitively on the directed edges (called arcs) of X and that for each pair of arcs there is a unique automorphism mapping one to the other. It is interesting to note that the above question is equivalent to asking which of the graphs $\mathrm{H}(p, q, t)$ admit ½-arc-transitive line graphs (see Proposition 1.1 below). A complete answer to this question is given in this paper for a special class of torusenes, that is, for the cubic cyclic Haar graphs (certain cubic Cayley graphs of dihedral groups) - see the definition below.

It is well-known that symmetries in molecular graphs have a significant role in spectroscopy. For example, the graph-theoretic concepts of one-regularity and ½-arc-transitivity have their chemistry counterpart in the concept of chirality. Chirality of molecules can be measured by different techniques, for example, by circular dichroism spectroscopy. It is a form of light absorption spectroscopy that measures the difference in absorbance of right- and left-circularly polarized light by a substance. It could answer (without the knowledge of the exact 3D-structure) certain general aspects of molecular structure, such as, whether a molecule possesses a right- or left-handed helical conformation.

The directionality of chemical bonds originating from a given atom is usually described by hybrids-proper linear combinations of atomic orbitals situated on the atom under consideration. For instance, the so-called σ-bonding is usually attributed to their hybrids (which are pointed to each other along the bond). However, instead of a pair of hybrids one could also

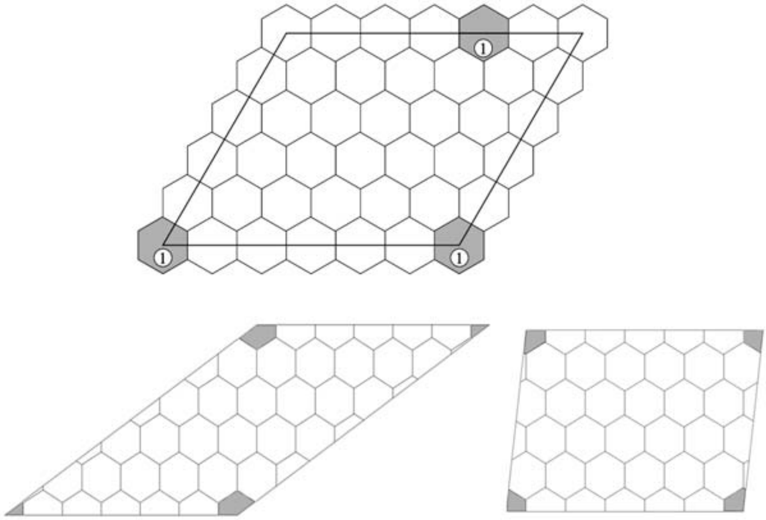

Figure 3. A torusene H(p, q, t) for p = 6, q = 5, t = 4. There are at least two possible ways of depicting H(p, q, t). One can take a parallelogram with the standard angle of 60° (in Refs. 2 and 3 the angle is 120°), identify its two lateral sides, and rotate the top side before identifying it with the bottom one. An alternative, depicted here twice, is to take a different parallelogram with the same bottom side as before in order to avoid rotations. Note that in the latter case the parallelogram is not unique.

describe the bonding by considering their symmetric linear combination. The combination is centered at the bond and is called a bond orbital. In graph-theoretic model a bond orbital is described by a vertex located at the σ-bond. Accordingly, the interaction of bond orbitals is described by the line graph of the original σ-skeleton graph. Such a model was introduced by Frost, Sandorfy, Polansky and others.

We wrap up this section with a short discussion of the various graph-theoretic concepts describing symmetry. As the main topic of this work touches several areas of mathematics, we have provided a collection of background references (see Refs. 10–15) in order to keep this paper of reasonable size.

We may consider the action of the automorphism group of a graph on various graph constituents. A graph is vertex-transitive and edge-transitive, respectively, provided its automorphism group acts transitively on the corresponding vertex set and edge set. An edge uv can be mapped to an edge xy in two possible ways; either by taking u to x and v to y, or u to y and v to x. An edge-transitive graph is arc-transitive if for any pair of edges both mappings are possible. A graph that is vertex- and edge- but not arc-transitive is called ½-arc-transitive. Note that there is a simple criterion for checking whether a vertex- and edge-transitive graph is ½-arc-transitive; namely, that is the case if and only if no automorphism of the graph interchanges the endvertices of some edge. Finally, a graph is 1-regular if the automorphism group acts regularly on the set of arcs.

Cubic vertex-transitive graphs fall naturally into three classes depending on the number of edge-orbits of the corresponding automorphism group. In case of three orbits, the graphs are called 0-symmetric (see Refs. 16 and 17). At the other extreme, if there is only one orbit, then the graph is arc-transitive. This follows from the fact that vertex-and edge-transitive graphs of odd valency are necessarily arc-transitive.[18]

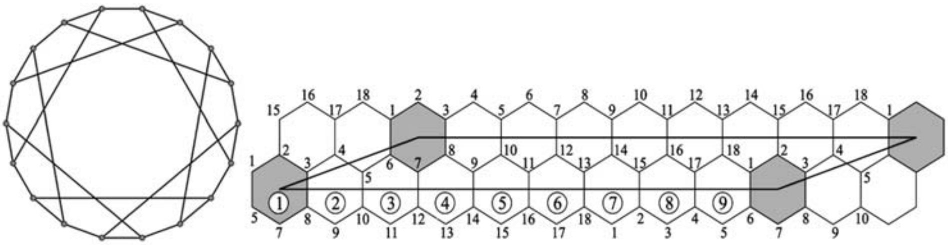

Figure 4. The smallest 0-symmetric graph Ha(261) has 18 vertices. Embedded on torus it gives rise to H(9, 1, 2).

The class of cubic arc-transitive graphs can be further refined by bringing into consideration the concept of k-arc-transitivity. Adopting the terminology of Tutte,[19] a k-arc in a graph X is a sequence of $k + 1$ vertices v_1, v_2,...,v_{k+1} of X, (not necessarily all distinct), such that any two consecutive terms are adjacent and any three consecutive terms are distinct. A graph X is said to be k-arc-transitive if the automorphism group of X, denoted Aut X, acts transitively on the set of k-arcs of X. By the well known result of Tutte,[19] a cubic arc-transitive graph is at most 5-arc-transitive, with the degree of transitivity having a reflection in the corresponding vertex stabilizers. For example if a cubic graph is 1-arc-transitive (but not 2-arc-transitive), then the corresponding vertex stabilizers are isomorphic to a cyclic group of order 3. In this case the automorphism group is regular on the set of 1-arcs, and the graph is 1-regular. Such graphs are of particular interest to us for their line graphs are tetravalent ½-arc-transitive graphs as is seen by the following result. Recall that the vertices of the line graph L(X) of a graph X are the edges of X, with adjacency corresponding to the incidence of edges in X.

Proposition 1. (Ref. 20, Proposition 1.1.) *A cubic graph is 1-regular if and only if its line graph is a tetravalent ½-arc-transitive graph.*

The Cayley graph Cay (G, S) of a group G with respect to a set of generators $S = S^{-1}$ has vertex set G with two vertices $g, g' \in G$ adjacent if and only if $g' = gs$ for some $s \in S$. We shall be interested in a particular class of Cayley graphs of dihedral groups arising from a set of generators all of which are reflections. For an integer n, a subset $S \subseteq \mathbb{Z}_n \backslash \{0\}$, the Cayley graph of a dihedral group D_{2n} with presentation $\langle a,b : a^n = 1,\ b^2 = 1, (ab)^2 = 1 \rangle$, relative to the set of generators $\{ab^s : s \in S\}$, may be represented as the graph with vertices u_i, $i \in \mathbb{Z}_n$ and v_i, $i \in \mathbb{Z}_n$, and edges of the form $u_i v_{i+s}$, $s \in S$, $i \in \mathbb{Z}_n$. The notation Dih (n, S) will be used for this graph. Note that the regular dihedral group is generated by the permutations ρ and τ mapping according to the respective rules

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

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

An alternative description for the graph Dih(n,S) puts it in a one-to-one correspondence with a positive integer N *via* its binary notation:

$$N = b_0 2^{n-1} + \cdots + b_{n-2}2 + \mathrm{b}_{n-1}$$

by letting $s \in S$ if and only if $b_s = 1$. Such a graph is referred to as the *cyclic Haar graph* Ha(N) of N (see Ref. 21).

As mentioned above, our attention will be focused to cubic (cyclic Haar) graphs Dih (n,S). We shall identify among them those which are 1-regular and thus give rise to tetravalent ½-arc-transitive graphs (Theorem 2.1).

CLASSIFICATION AND CONSEQUENCES

We say that two subsets S and T of $\mathbb{Z}_n$ are equivalent and write $S \sim T$ if there are $a \in \mathbb{Z}_n^*$ and $b \in \mathbb{Z}_n$ such that $T = aS + b$. Clearly, Dih$(n,S) \cong$ Dih (n,T) if S and T are equivalent. The result below classifies cubic arc-transitive graphs Dih(n,S). (A note for readers with a non-mathematical background: arithmetic operations are to be taken mod n if at least one argument is from $\mathbb{Z}_n$. However the symbol mod n is always omitted, the ring $\mathbb{Z}_n$ being clear from the context. This should cause no confusion.)

Theorem 1. *Let* n *be a positive integer and* $\mathrm{S} = \{i, j, k\}$ *be a subset of* $\mathbb{Z}_n$ *such that the graph* $X = Dih(\mathrm{n}, S)$ *is connected and arc-transitive. Then one of the following occurs*:

(*i*) $X \cong K_{3,3} \cong Dih(3,\{0,1,2\})$ *and is 3-arc-transitive; or*

(*ii*) *X is isomorphic to the cube* $Q_3 \cong K_{4,4} - 4K_2 \cong Dih\ (4,\{0,1,2\})$ *and is 2-arc-transitive; or*

(*iii*) *X is isomorphic to the Heawood graph* $Dih\ (7,\{0,1,3\})$ *and is 4-arc-transitive; or*

(*iv*) *X is isomorphic to the Möbius-Kantor graph* $Dih\ (8,\{0,1,3\})$ *and is 2-arc-transitive; or*

(*v*) $n \geq 11$ *is odd and there exists a nonidentity element* $r \in \mathbb{Z}_n^*$ *such that* $r^2 + r + 1 = 0$, $S \sim \{0,1,r+1\}$ *and* $X \cong Dih(n,\{0,1,r+1\})$ *is 1-regular and its line graph is a tetravalent ½-arc-transitive graph.*

PROOF. Let $\Delta(S) = \{j-i,\ k-j,\ i-k\}$ be the difference set of S. Since X is connected, it follows that

$$\langle \Delta(S) \rangle = \mathbb{Z}_n, \tag{3}$$

We may think of the edges of the graph X as being »colored« with colors i, j and k. We are going to distinguish two different cases.

CASE 1: X has girth 4.

Depending on the color distribution, there can be two essentially different types of 4-cycles in X. More precisely, the color distribution is either of the form *xyxy* or of the form *xyxz*, where $x,y,z \in \{i,j,k\}$ are all distinct. However, because of arc-transitivity the colors i,j,k must be uniformly distributed on all 4-cycles of X. This implies that either $2(x-y) = 0$ for any two distinct $x,y \in \{i,j,k\}$, which is not possible, or alternatively, X contains 4-cycles of the second type. But then with no loss of generality $j + k = 2i$. Hence S is equivalent to the set $\{0,i,2i\} = S - k$. Again arguing on the equal color distribution, it may be seen that either $i \in \{\frac{n}{3},\frac{2n}{3}\}$ and $X \cong K_{3,3}$ (see Figure 5) or else $i \in \{\frac{n}{4},\frac{3n}{4}\}$ and $X \cong Q_3$ (see Figure 6).

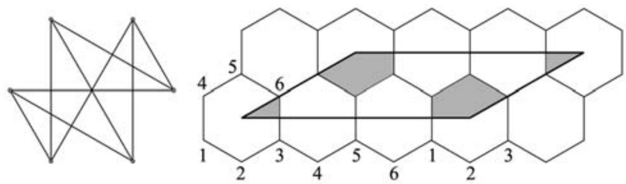

Figure 5. The complete bipartite graph $K_{3,3}$ or H(3,1,1).

CASE 2. X has girth 6.

Note that there are »generic« 6-cycles in X with color distribution *ijkijk*, a typical representative being the cycle $u_0 w_i u_{i-j} w_{i-j+k} u_{k-j} w_j u_0$.

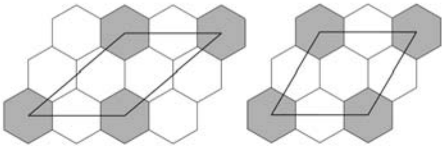

Figure 6. Two inequivalent embeddings H(2,2,1) and H(2,2,0) (as maps on the torus) of the same graph, the cube Q_3. This is the only case where a toroidal map is not determined by its graph.

Suppose first that there are also non-generic 6-cycles in X. Then with no loss of generality, we must have a 6-cycle in X with, say, color distribution *jijijk*, and then since each color must lie on the same number of different 6-cycles, X must also contain 6-cycles having color distributions *kjkjki* and *ikikij*, or else 6-cycles with color distribution *jkjkji*.

In the first case, $3j = 2i + k$, $3k = 2j + i$ and $3i = 2k + j$. It follows that $7(j - i) = 7(k - j) = 7(i - k) = 0$. If 7 is co-prime with n, then $i = j = k$, which is impossible. Thus 7 divides n. This together with (3) implies that $n = 7$ is the only possibility. It is easily seen that $aS + b = \{0,1,3\}$ for some $a \in \mathbb{Z}_7^*$ and $b \in \mathbb{Z}_7$, implying that X is isomorphic to the Heawood graph (see Figure 2).

In the second case, $3j = 2i + k$ and $3k = 2i + j$. It follows that $8(j - i) = 8(k - j) = 8(i - k) = 0$. If 8 is co-prime with n, that is if n is odd, then $i = j = k$, which is impossible. Thus n is even. This together with (3) implies that $n = 8$ is the only possibility. It is easily seen that $aS + b = \{0,1,3\}$ for some $a \in \mathbb{Z}_8^*$ and $b \in \mathbb{Z}_8$, implying that X is isomorphic to the Möbius-Kantor graph Dih(8,{0,1,3}) (see Figure 7).

We may therefore assume that the generic 6-cycles above are the only 6-cycles in X. As a consequence, the three color classes $\{i,j,k\}$ of edges in X are blocks of imprimitivity for Aut X. We now use this fact to prove that the normalizer of the cyclic group $\langle\rho\rangle$ of order n contains an element of order 3. We argue as follows. Let σ be an automorphism of order 3 in the stabilizer of u_0 cyclically permuting the three neighbors v_i, v_j and v_k. We claim that σ normalizes ρ. Now $\rho^\sigma = \sigma^{-1}\rho\sigma$ fixes the three color classes i, j and k. Then there exists $r \in \mathbb{Z}_n^*$ such that $\gamma = \rho^{-r}\rho^\sigma$ fixes two adjacent vertices and of

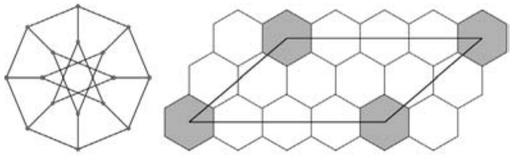

Figure 7. The Möbius-Kantor graph H(4,2,1).

course all of the color classes. The connectedness of X implies $\gamma = 1$ and so $\rho^\sigma = \rho^r$. We now use the action of the group $\langle \rho,\sigma \rangle$ to show that $aS + b = \{0,1,r+1\}$ for some $a \in \mathbb{Z}_n^*$ and $b \in \mathbb{Z}_n$.

Since $\rho^\sigma = \rho^r$ it may be deduced that

$$u_i\sigma = u_{ri} \text{ for each } i \in \mathbb{Z}_n \tag{4}$$

As for the action of σ on the three neighbors of u_0, we have that σ either fixes all of them, which may be easily seen to lead to a contradiction, or it permutes them cyclically in the order v_i, v_j v_k. Therefore if, given a subset $A \subseteq \mathbb{Z}_n$, we let u_A denote the set $\{u_a : a \in A\}$, then σ cyclically permutes the sets of neighbors $N(v_i) = u_{-S+i}$, $N(v_j) = u_{-S+j}$, and $N(v_k) = u_{-S+k}$. Consequently, $-rS + ri = -S + j$, $-rS + rj = -S + k$ and $-rS + rk = -S + i$. By computation, $r(j-i) = k - j$, $r(k-j) = i - k$ and $r(i-k) = j - i$. It follows that

$$(r^2 + r + 1)(j - i) = 0. \tag{5}$$

Moreover, $k = j + r(j-i)$ and so $S = \{i, j, j + r(j-i)\}$. *Thus* $\Delta(S) = \{j-i, r(j-i), (r+1)(j-i)\}$ and $(j-i)$ is co-prime with n, by (3). But then $r^2 + r + 1 = 0$ by (5). In particular, $r + 1 \in \mathbb{Z}_n^*$, forcing n to be odd. Furthermore, as $(j-i) \in \mathbb{Z}_n^*$ too, we have that $S \sim \{0,1,r+1\} = (j-i)^{-1}(S-i)$. In particular we have that $n \geq 13$, since for $n = 7$ we have the above Heawood graph, whereas for $n = 9$ the above condition (5) is not satisfied for any $r \in \mathbb{Z}_9^*$.

As for 1-regularity of X, and consequently, in view of Proposition 1, the ½-arc-transitivity of its line graph L(X), recall that the generic 6-cycles are the only 6-cycles in X. Consequently X is at most 1-arc-transitive and hence in view of Tutte's theory,[19] 1-regular. This completes the proof of Theorem 1. Note that the corresponding vertex stabilizers in Dih(n,S) and L(Dih(n,S)) are isomorphic, respectively, to $\mathbb{Z}_3$ and $\mathbb{Z}_2$. As a final remark, observe that the line graph L(Dih(n,$\{0,1,r+1\}$)) is isomorphic with the graph M(r;3,n) introduced in Ref. 22, where its ½-arc-transitivity is proved for all integers $n \geq 9$ for which 3 divides the Euler function $\phi(n)$.

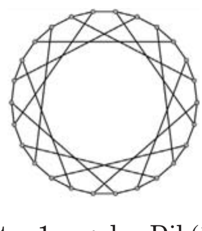

Figure 8. For $n = 13$, $r = 3$, we get a 1-regular Dih(13, $\{0,1,4\}$) which is the graph 26 from the Foster census and can be generated by the LCF-code (7,–7).[1]

TABLE I

Small values of n and r, such that $r^2 + r + 1 = 0 \pmod n$. The graphs M(n,r) are 1-regular except for the first two entries where we get M(3,1) = $K_{3,3}$ and M(7,2) which is the well-known Heawood graph; see Figure 2. The fourth column refers to notation from Ref. 24.

	n	r	a		n	r	a		n	r		n	r
1	3	1	6	31	163	58	326	61	327	154	91	487	232
2	7	2	14	32	169	22	338A	62	331	31	92	489	58
3	13	3	26	33	181	48	362	63	337	128	93	499	139
4	19	7	38	34	183	13	366	64	343	18	94	507	22
5	21	4	42	35	193	84	386	65	349	122	95	511	81
6	31	5	62	36	199	92	398	66	361	68	96	511	137
7	37	10	74	37	201	37	402	67	367	83	97	523	60
8	39	16	78	38	211	14	422	68	373	88	98	541	129
9	43	6	86	39	217	25	434A	69	379	51	99	543	229
10	49	18	98	40	217	67	434B	70	381	19	100	547	40
11	57	7	114	41	219	64	438	71	397	34	101	553	23
12	61	13	122	42	223	39	446	72	399	121	102	553	102
13	67	29	134	43	229	94	458	73	399	163	103	559	165
14	73	8	146	44	237	55	474	74	403	87	104	559	178
15	79	23	158	45	241	15	482	75	403	191	105	571	109
16	91	9	182B	46	247	18	494A	76	409	53	106	577	213
17	91	16	182A	47	247	87	494B	77	417	181	107	579	277
18	93	25	186	48	259	100		78	421	20	108	589	87
19	97	35	194	49	259	121		79	427	74	109	589	273
20	103	46	206	50	271	28		80	427	135	110	597	106
21	109	45	218	51	273	16		81	433	198	111	601	24
22	111	10	222	52	273	100		82	439	171	112	607	210
23	127	19	254	53	277	116		83	453	118	113	613	65
24	129	49	258	54	283	44		84	457	133	114	619	252
25	133	11	266B	55	291	61		85	463	21	115	631	43
26	133	30	266A	56	301	79		86	469	37	116	633	196
27	139	42	278	57	301	135		87	469	163	117	637	165
28	147	67	294B	58	307	17		88	471	169	118	637	263
29	151	32	302	59	309	46		89	481	100	119	643	177
30	157	12	314	60	313	98		90	481	211	120	651	25

a = Ref. 24.

The graphs in cases (*iii*), (*iv*) and (*v*) of the above theorem have girth 6. Such bipartite graphs arise from configurations and are known as Levi graphs of n_3-configurations. For instance, the Heawood graph is the Levi graph of a well-known Fano configuration, and the graph Dih(8,{0,1,3}) (isomorphic to the generalized Petersen graph GP(8,3) Ref. 23) is the Levi graph of the Möbius-Kantor configuration. Since the graphs in case (*v*) are 1-regular, the corresponding configurations are point-, line- and flag-transitive; more precisely, flag-regular. Moreover, as there is an involution interchanging the two sets of bipartition, the corresponding configurations are also self-polar. All of the graphs in Theorem 1 form an infinite class $\mathrm{X}(n,r) \cong \mathrm{Dih}\,(n, \{0,1,r+1\})$, where, in cases (*iii*) and (*v*), we have $r \in \mathbb{Z}_n^*$ satisfying $r^2 + r + 1 = 0$. These graphs may all be described by the LCF-code $(2r+1, -2r-1)^n$. Note that in case (*v*) the full automorphism group is isomorphic to the semidirect product $\mathbb{Z}_n \rtimes \mathbb{Z}_6$. The first 47 graphs $\mathrm{X}(n,r)$ of small order can be found in the Foster Census (see Ref. 24. and Table I).

Also, we remark that the hexagonal toroidal embeddings of $\mathrm{X}(n,r)$ in cases (*i*), (*iii*), and (*v*) require a single row of hexagons and the corresponding map can be described as $\mathrm{H}(n,1,n-r-2)$. As for cases (*ii*) and (*iv*) see Figures 6 and 7.

Furthermore the line graphs of graphs $\mathrm{X}(n,r)$ in case (*v*) are, as noted above, ½-arc-transitive. They belong to the class of tetravalent ½-arc-transitive graphs $\mathrm{M}(r;3,n)$ from Ref. 22. The latter may be found as members of a more general class of the so called tightly attached graphs in the Vega Package and Vega Graph gallery available at the address: http://vega.ijp.si.

The graph 56A is the smallest 1-regular graph in the Foster census[24] that is not covered by our Theorem 1. The line graph of the graph 26 in line 3 of our table is the smallest tetravalent ½-arc-transitive graph of girth 3, see Figure 8.

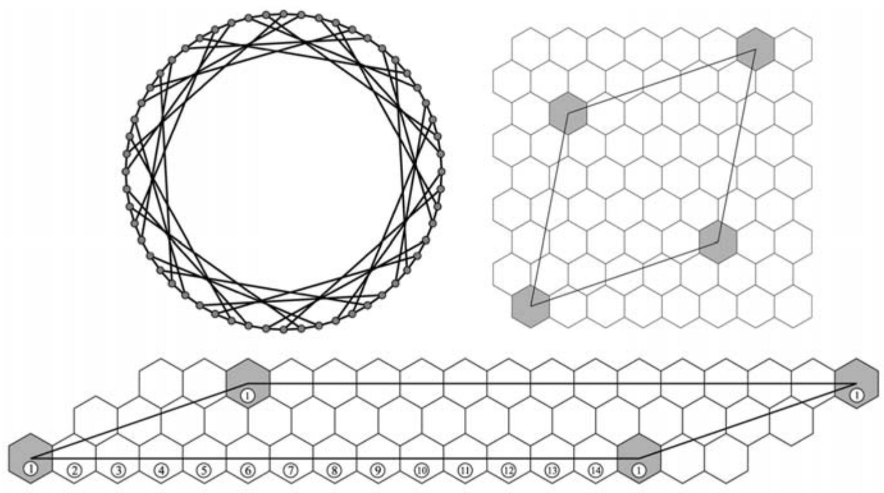

Figure 9. The smallest 1-regular hexagonal torusene H(14,2,4), not covered by our Theorem 1, denoted as 56A in the Foster Census;[24] compare Figure 1.

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SAŽETAK

Simetrije heksagonskih molekulskih grafova na torusu

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Poučavana su simetrijska svojstva nekih molekulskih grafova na torusu. Utvrđeno je koji su kubični ciklički Haarovi grafovi 1-regularni, što je ekvivalentno iskazu da su njihovi linijski grafovi ½-arc-tranzitivni. Iako te simetrije onemogućuju razlikovanje svih vrhova i svih bridova, one uključuju svojstvenu kiralnost odgovarajućih molekulskih grafova.