Analysis of the Relationship among the Graphs Isomorphic to Multilayered Cyclic Fence Graphs (MLCFG)

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Multilayered cyclic fence graphs (MLCFG, $E_{m,n}$, $F_{m,n}$, $D_{m,n}$, $G_{m,n}$, $X_{m,n}$) are proposed to be defined, all of which are composed of *m* 2*n*-membered cycles with periodic bridging. They are also cubic and bipartite. Hamiltonian wheel graph, H $(n,\{j_k\})$, and parallelogram-shaped polyhex graph are also defined. All the members of MLCFGs are found to be isomorphic to the so-called "torus benzenoid graphs", while some members of MLCFGs are found to be related to the Hamilton wheel graphs. Through the construction of Hamilton wheel graph and the matrix representation by Kirby, a number of isomorphic relations among MLCFGs, Hamilton wheel graphs, and polyhex graphs were obtained. These relations among the MLCFG members were found also by the help of the characteristic quantities of MLCFGs.

1. INTRODUCTION

Hosoya and Harary defined the cyclic fence graph, $F_{1,n}$, which is composed of *n* bars and *n* pairs of crossing bridges, as shown in Figure 1.[1] All these $F_{1,n}$'s are cubic and bipartite and are found to be closely related to the graphs composed of only hexagons, especially through the number of perfect matching, or Kekulé number, $K(G)$. As an extension of the cyclic fence graph, a multilayered cyclic fence graph (MLCFG) is constructed by piling up the cycle graph as in Figure 2.[2,3] All the members of MLCFGs which are also cubic and bipartite are found to be isomorphic to the so-called "torus benzenoid graphs" which can be constructed by regular cyclization of polyhex graphs. By a polyhex graph here we mean any structure obtained by fusing hexagons. By a toroidal polyhex we mean a structure that can be mapped as a boundless polyhex on the surface of a torus.[4−6] MLCFGs have many interesting chemical features. For example, even their smaller members with less than a hundred vertices can reproduce the characteristic features of the electronic structure of the infinitely large graphite network. Recently a number of chemistry papers dealing with toroidal polyhexes are rapidly increasing.[4−13] On the other hand, from the graph-theoretical viewpoint, the series of MLCFGs are found to be transformed into widely known graphs in the graph-theory, such as the Hamilton wheel graph.[3]

Since the properties of the two series of MLCFGs, $E_{m,n}$ and $F_{m,n}$ (see Figure 2) have already been reported,[3] in this paper some new findings of the $D_{m,n}$, $G_{m,n}$, $X_{m,n}$ graphs will be presented, with particular reference to the isomorphic relations among MLCFGs, Hamilton wheel graphs, and polyhex graphs.[14−16] Mathematical features of MLCFGs might have some crucial role in analyzing the reaction graphs which Balaban and others have proposed for discussing the complexity of chemical reactions and related phenomena.[17−21]

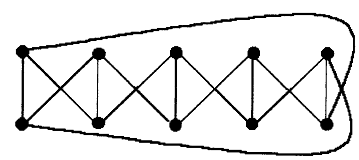

Figure 1. $F_{1,5}$.

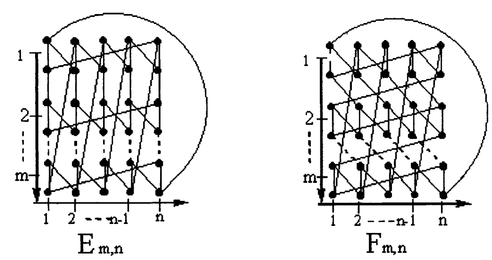

Figure 2. $E_{m,n}$ and $F_{m,n}$ families.

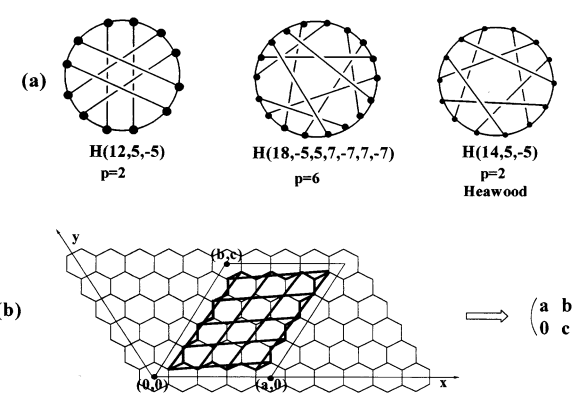

Figure 3. (a) Hamilton wheel graph and (b) P-graph.

2. DEFINITIONS

For recognizing the symmetry of these families of graphs, the "Hamilton wheel graph", H $(n,\{j_k\})$, has been defined,

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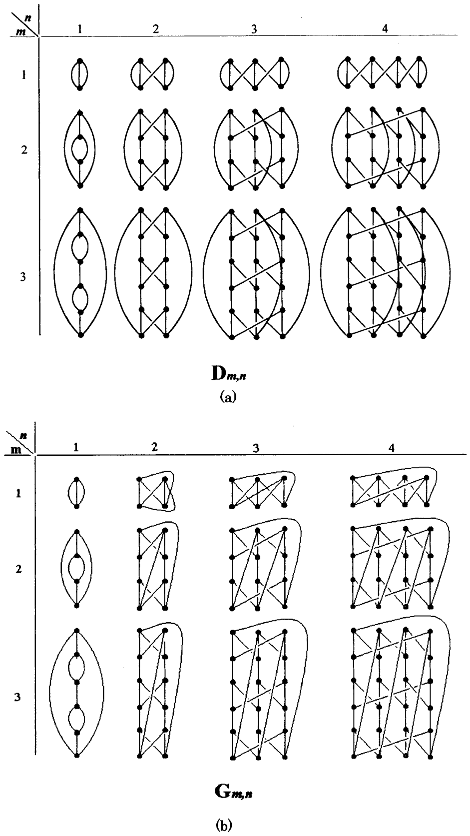

Figure 4. Lower members of (a) $D_{m,n}$ and (b) $G_{m,n}$ families.

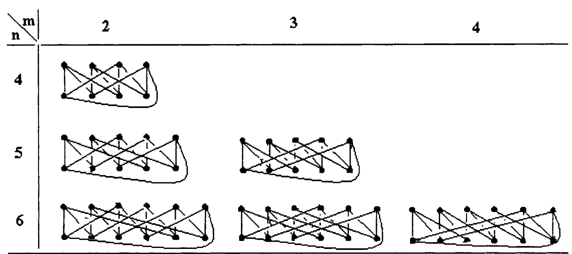

Figure 5. Lower members of $X_{m,n}$ family.

whose vertices are lying on an n-membered cyclic graph, C_n. First the H (n, j) graph is constructed from C_n by

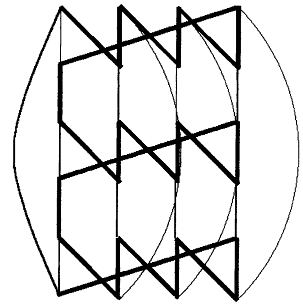

Figure 6. Hamilton circuit of $D_{3,4}$ graph.

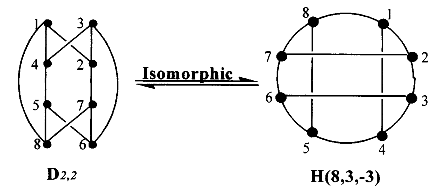

Figure 7. The isomorphic relation between $D_{2,2}$ graph and H(8,3,−3).

connecting each of the component vertices to the vertex located at its clockwise jth neighbor. Then a p-cyclic Hamilton wheel graph, H (n,{j_k}) with $k = 1,2,...,p$, is constructed by p-periodic,{j_k}-joinings of the n vertices of C_n as in Figure 3a. In this notation the so-called Heawood graph[3] or the six-cage is represented by H(14,5,−5), which, however, is not directly related to any of MLCFG.[3] The $D_{m,n}$ and $G_{m,n}$ graphs are defined as in Figure 4. All these MLCFGs are composed of m $2n$-membered cycle graphs with periodic bridging and can be mapped without edge crossing on a surface of a donut and thus can be grouped into torus graphs with genus one. We also define a series of cyclic graphs, $X_{m,n}$ derived from a $2n$-membered cycle graph with m-step periodic cross-bridging as in Figure 5.

The name of Hamilton wheel graph comes from the Hamiltonian circuit. Namely, one can trace a single stroke of a brush through all the vertices along the circle. For later discussions the following relations, though formal, will be shown to be effective for recognizing the isomorphic relation

Table 1. Isomorphism between the Hamilton Wheel Graphs and $D_{m,n}$ Family[a]

	m				
n	**1**	**2**	**3**	**4**	**5**
1	H(2,1)	H(4,1,−1)	H(6,1,−1)	H(8,1,−1)	H(10,1,−1)
2	H(4,1,−1)	*H(8,3,−3)*	H(12,5,−5)	H(16,−3,3,5,−5)	H(20,9,−9)
3	H(6,1,−1)	H(12,5,−5)	*H(18,−5,5,7,−7,7,−7)*	H(24,7, −7)	H(30,11,−11)
4	H(8,1,−1)	H(16,7,−7)	H(24,7,−7)	H(32,−7,7,9,−9,9,−9,9,−9)	H(40,9,−9)
5	H(10,1,−1)	H(20,9,−9)	H(30,11,−11)	H(40,9,−9)	H(50,−9,9,11,−11,11,−11,11, −11,11,−11)
6	H(12,1,−1)	H(24,11,−11)	H(36,−5,5,7,−7,7,−7)	H(48,−11,11,13,−13,13,−13,13, −13,13,−13,13,−13)	H(60,11,−11),
7	H(14,1,−1)	H(28,13,−13)	H(42,13,−13)	H(56,15,−15)	H(70,29,−29)
8	H(16,1,−1)	H(32,15,−15)	H(48,17,−17)	H(64,−15,15,17,−17, 17,−17, 17, −17,17,−17, 17,−17, 17,−17, 17,−17)	H(80,31,−31)
9	H(18,1,−1)	H(36,17,−17)	H(54,−5,5,7,−7,7,−7)	H(72,17,−17)	H(90,19,−19)
10	H(20,1,−1)	H(40,19,−19)	H(60,19,−19)	H(80,−19,19,21,−21, 21,−21, 21, −21,21,−21, 21,−21, 21,−21, 21,−21,21,−21, 21,−21)	H(100,−9,9,21,−21, 21,−21, 21, −21, 21,−21, 21,−21, 21,−21, 21,−21, 21,−21, 21,−21)

[a] Italic, vertex and edge topicities are both unity.

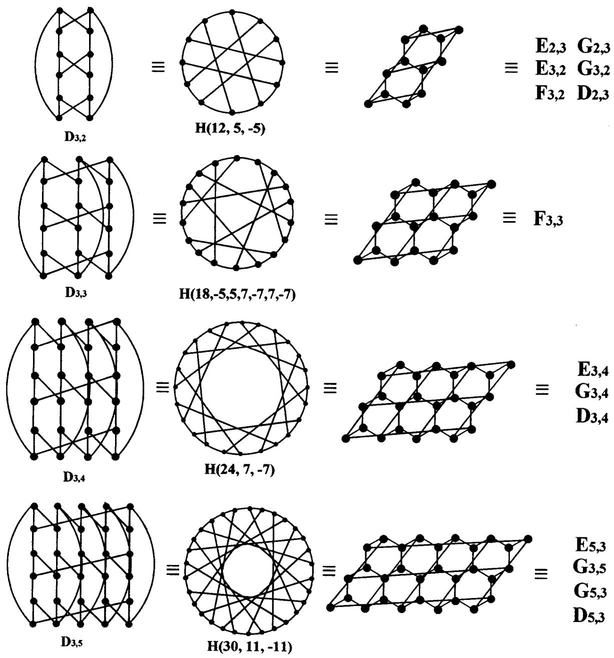

Figure 8. Isomorphism of $D_{m,n}$ graphs.

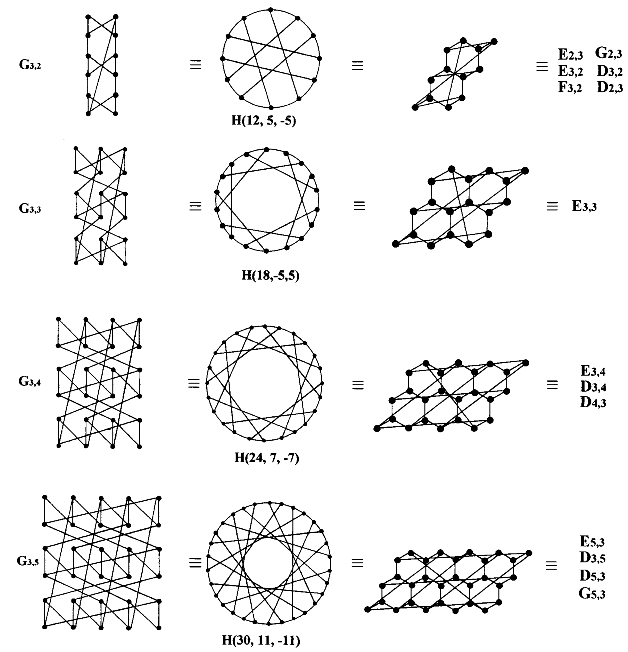

Figure 9. Isomorphism of $G_{m,n}$ graphs.

among the Hamilton wheel graphs.

$$H(n,j,k) = H(n,k,j) = H(n,-j,-k) = H(n,-k,-j) \quad (1)$$

$$H(n,j,k) = H(n,j \pm n,k) = H(n,j,k \pm n) \quad (2)$$

To discuss isomorphic relations among polyhex graphs and MLCFGs, the matrix representation by Kirby was utilized[4−6] (see Figure 3b). Namely, a parallelogram-typed polyhex graph (P-graph) can be determined by the three vertices, (0, 0), (a, 0), and (b, c), representing the key hexagons and mapped on the skewed 2-dimensional coordinate system proposed by Kirby. Then this P-graph is denoted by the following 2 × 2 matrix

$$\begin{pmatrix} a & b \\ 0 & c \end{pmatrix}$$

3. ISOMORPHISM

For systematic analysis of graphs, the characteristic quantities of the graph play extremely important roles. They are nonadjacent number, adjacency matrix, topological index, matching polynomial. When a pair of graphs were found to have exactly the same sets of these characteristic quantities, close examination of the adjacency relations among the vertices was reformed to check their isomorphism. Then we could find various kinds of isomorphic relations for $D_{m,n}$, $G_{m,n}$, $X_{m,n}$ graphs. The relations of those MLCFGs with Hamilton wheel graphs and P-graphs and the relations among MLCFGs will also be discussed.

3.1. The Relatonship between MLCFGs and Hamilton Wheel Graphs. $D_{m,n}$ Family. By noticing its construction scheme, any member of $D_{m,n}$ family is found to have a Hamilton circuit (see Figure 6). Namely, by traversing along the top row one can move down to the next row step by step and finally come back again the starting point to form a Hamilton circle. The double layered cyclic fence graph $D_{2,n}$ can be transformed into their corresponding Hamilton wheel graph, H(4n, 2n−1, −(2n−1)). For example, $D_{2,2}$ graph holds exactly the same neighboring relations with the vertices of H(8,3,−3) (see Figure 7).

The isomorphic relations between the lower members of $D_{m,n}$ family and Hamilton wheel graphs are shown in Table 1, which are exemplified in Figure 8. All the $D_{m,n}$ graphs were found to be isomorphic to some of the Hamilton wheel graphs. At first sight except for the $D_{2,n}$ series no simple relation can be detected. However, we could find three

Table 2. Isomorphism between the Hamilton Wheel Graph and $G_{m,n}$ Family[a]

	m				
n	1	2	3	4	5
1	H(2,1)	H(4,1,−1)	H(6,1,−1)	H(8,1,−1)	H(10,1,−1)
2	H(4,1,−1)	*H(8,3,−3)*	H(12,5,−5)	H(16,7,−7)	H(20,9,−9)
3	H(6,3,−3)	H(12,5,−5)	H(18,5,−5)	H(24,9,−9)	H(30,11,−11)
4	H(8,3,−3)	H(16,3,−3)	H(24,7,−7)	H(32,7,−7)	H(40,11,−11)
5	H(10,3,−3)	H(20,9,−9)	H(30,11,−11)	H(40,15,−15)	H(50,11,−11)
6	H(12,3,−3)	H(24,5,−5)	H(36,5,−5)	H(48,9,−9)	*b*
7	H(14,3,−3)	H(28,7,−7)	H(42,5,−5)	H(56,15,−15)	H(70,29,−29)
8	H(16,3,−3)	H(32,13,−13)	H(48,17,−17)	H(64,23,−23)	H(80,11,−11)
9	H(18,3,−3)	H(36,7,−7)	H(54,7,−7)	H(72,33,−33)	H(90,19,−19)
10	H(20,3,−3)	H(40,11,−11)	*b*	H(80,11,−11)	H(100,9,−9)

[a] Italic, vertex and edge topicities are both unity. [b] No corresponding Hamilton wheel graph.

Table 3. Isomorphism between the Hamilton Wheel Graph and $X_{m,n}$ Family

	m					
n	2	3	4	5	6	7
4	H(8,5,−5)					
5	H(10,5,−5)	H(10,7,−7)				
6	H(12,5,−5)	H(12,7,−7)	H(12,9,−9)			
7	H(14,5,−5)	H(14,7,−7)	H(14,9,−9)	H(14,11,−11)		
8	H(16,5,−5)	H(16,7,−7)	H(16,9,−9)	H(16,11,−11)	H(16,13,−13)	
9	H(18,5,−5)	H(18,7,−7)	H(18,9,−9)	H(18,11,−11)	H(18,13,−13)	H(18,15,−15)
10	H(20,5,−5)	H(20,7,−7)	H(20,9,−9)	H(20,11,−11)	H(20,13,−13)	H(20,15,−15)

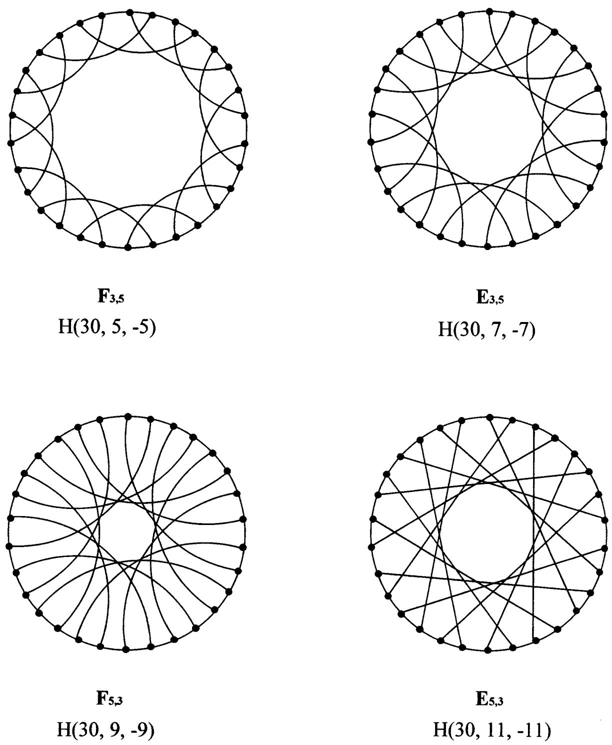

Figure 10. Mapping of Hamilton wheel graphs.

different sets of general correlation relations up to $m = 4$ as follows.

$$D_{1,n} = H(2n,1,-1)\ (n \geq 1) \tag{3}$$

$$D_{2,n} = \mathrm{H}(4n,(2n-1),-(2n-1))\ (n \geq 1) \tag{4}$$

$$\begin{cases} D_{3,3-n} = \mathrm{H}(6(3n-1),(6n-1),-(6n-1)) & (n \geq 1) \\ D_{3,3n+1} = \mathrm{H}(6(3n+1),(6n+1),-(6n+1)) & (n \geq 0) \\ D_{3,3n} = \mathrm{H}(18n,-5,5,7,-7,7,-7) & (n \geq 1) \end{cases} \tag{5}$$

$$\begin{cases} D_{4,4n+1} = H(8(4n+1),(8n+1),-(8n+1)) & (n \geq 0) \\ D_{4,4n-1} = H(8(4n-1),(8n-1),-(8n-1)) & (n \geq 1) \\ D_{4,2n} = H(16n,-(4n-1),(4n-1),\underbrace{(4n+1),\ldots,-(4n+1)}_{2n-1} & (n \geq 1) \end{cases} \tag{6}$$

As the value of *m* increases regularity for the H expressions seemed to become much more complicated. It is difficult to give rigorous proofs for these relations. However, their validity can be assured from our long experience in this field.

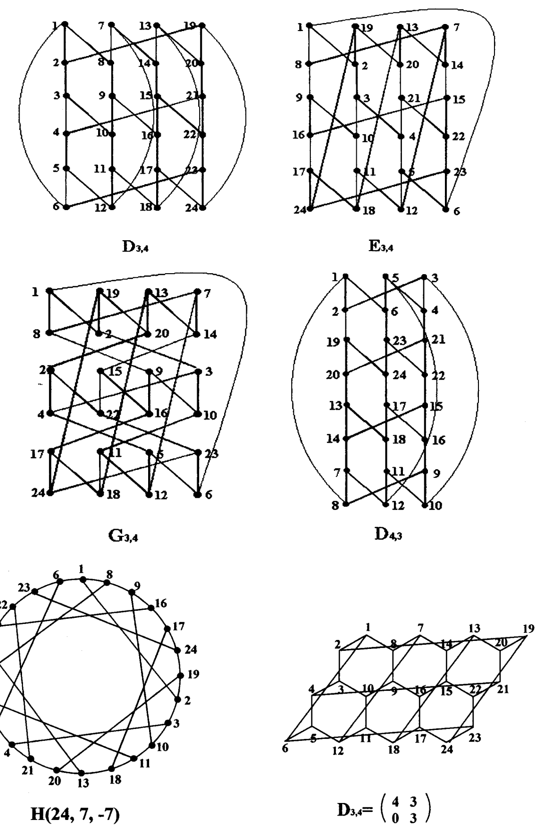

Figure 11. $D_{3,4}$, $E_{3,4}$, $G_{3,4}$, $D_{4,3}$.

$G_{m,n}$ Family. Contrary to the case of $D_{m,n}$ graphs, the isomorphic list for $G_{m,n}$ graphs to Hamilton wheel graphs in Table 2 seems to be much simpler and neater. Namely, each member of $G_{m,n}$ graphs can find its counterpart in the family of H(2*mn*, *k*,−*k*). Some of the isomorphic relations are shown in Figure 9.

It is interesting to observe the following relations

$$G_{2,2} = \mathrm{H}(8,3,-3),\ G_{3,2} = \mathrm{H}(12,5,-5),\ G_{4,2} = \mathrm{H}(16,7,-7) \tag{7}$$

or generally

$$G_{m,2} = \mathrm{H}(4m,(2m-1),-(2m-1))\ (m \geq 1) \tag{8}$$

However, for $G_{m,n}$ with larger *n*, many puzzling relations hard to be solved, are found as

$$G_{2,3} = \mathrm{H}(12,5,-5),\ G_{3,3} = \mathrm{H}(18,5,-5),\ G_{4,3} = \mathrm{H}(24,9,-9) \tag{9}$$

$$G_{2,4} = \mathrm{H}(16,3,-3),\ G_{3,4} = \mathrm{H}(24,7,-7),\ G_{4,4} = \mathrm{H}(32,7,-7) \tag{10}$$

Table 4. Isomorphism of $D_{m,n}$

	m		
n	2	3	4
2	$E_{2,2}$, $F_{2,2}$, $G_{2,2}$	$E_{2,3}$, $E_{3,2}$, $F_{3,2}$, $G_{2,3}$, $G_{3,2}$, $D_{2,3}$	$E_{4,2}$, $F_{2,4}$, $F_{4,2}$, $G_{4,2}$, $D_{2,4}$
3	$E_{2,3}$, $E_{3,2}$, $F_{3,2}$, $G_{2,3}$, $G_{3,2}$, $D_{3,2}$	$F_{3,3}$	$E_{3,4}$ $G_{3,4}$, $D_{4,3}$
4	$E_{4,2}$, $F_{2,4}$, $F_{4,2}$ $G_{4,2}$, $D_{4,2}$	$E_{3,4}$, $G_{3,4}$, $D_{4,3}$	$F_{4,4}$
5	$E_{5,2}$, $F_{5,2}$, $G_{2,5}$, $G_{5,2}$, $D_{5,2}$	$E_{3,5}$, $G_{3,5}$, $G_{5,3}$, $D_{5,3}$	$E_{4,5}$, $D_{5,4}$
6	$E_{6,2}$, $F_{6,2}$, $G_{6,2}$	$F_{3,6}$, $F_{6,3}$	$F_{6,4}$
7	$E_{7,2}$, $F_{7,2}$, $G_{7,2}$	*b*	$E_{7,4}$, $G_{7,4}$
8	$E_{8,2}$, $F_{8,2}$, $G_{8,2}$	$E_{8,3}$, $G_{3,8}$, $G_{8,3}$	*b*

[b] No corresponding graphs.

Table 5. Isomorphism of $G_{m,n}$

	m		
n	2	3	4
2	$E_{2,2}$, $F_{2,2}$, $D_{2,2}$	$E_{2,3}$, $E_{3,2}$, $F_{3,2}$ $D_{2,3}$, $D_{3,2}$, $G_{2,3}$	$E_{4,2}$, $F_{2,4}$, $F_{4,2}$ $D_{2,4}$, $D_{4,2}$
3	$E_{2,3}$, $E_{3,2}$, $F_{3,2}$ $D_{2,3}$, $D_{3,2}$, $G_{3,2}$	$E_{3,3}$	$E_{4,3}$, $F_{4,3}$
4	$E_{1,8}$	$E_{3,4}$, $D_{3,4}$, $D_{4,3}$	$E_{4,4}$
5	$E_{5,2}$, $F_{5,2}$ $D_{2,5}$, $D_{5,2}$, $G_{5,2}$	$E_{5,3}$ $D_{3,5}$, $D_{5,3}$, $G_{5,3}$	$F_{4,5}$
6	$E_{2,6}$, $F_{3,4}$	$E_{2,9}$	*a*
7	$F_{2,7}$	*a*	$E_{7,4}$, $G_{7,4}$
8	*	$E_{8,3}$ $D_{3,8}$ $G_{8,3}$	*a*

[a] No corresponding graphs.

At this stage, except for eq 8, it is rather difficult to deduce general rules for the isomorphism between the $G_{m,n}$ ($n>0$) family and Hamilton wheel graphs.

$X_{m,n}$ Family. Since the topological structure of $X_{m,n}$ graphs are simple, the isomorphic relations between Hamilton wheel graphs and $X_{m,n}$ family are rather regular as seen in Table 3. They can be formulated into the following expression.

$$X_{m,n} = H(2n, (2m+1), -(2m+1)) \ (m \geq 1) \qquad (11)$$

Table 6. Isomorphism of $X_{m,n}$

	m			
n	2	3	4	5
4	$E_{1,4}$, $E_{2,2}$, $F_{2,2}$ $G_{2,2}$, $D_{2,2}$			
5	$E_{1,5}$ $X_{3,5}$	$E_{1,5}$ $X_{2,5}$		
6	$E_{2,3}$, $E_{3,2}$, $F_{3,2}$, $X_{3,6}$ $D_{2,3}$, $D_{3,2}$, $G_{3,2}$, $G_{2,3}$	$E_{2,3}$, $E_{3,2}$, $F_{3,2}$, $X_{2,6}$ $D_{2,3}$, $D_{3,2}$, $G_{3,2}$, $G_{2,3}$	$F_{2,3}$	
7	$X_{4,7}$	$E_{1,7}$ $X_{5,7}$	$X_{2,7}$	$X_{3,7}$
8	$E_{4,2}$ $X_{3,8}$	$E_{2,4}$ $X_{2,8}$	$E_{4,2}$ $X_{3,8}$	$E_{2,4}$ $X_{2,8}$
9	$E_{3,3}$, $G_{,3,3}$ $X_{3,9}$, $X_{5,9}$	$E_{3,3}$, $G_{,3,3}$ $X_{2,9}$, $X_{5,9}$	$E_{1,9}$	$E_{3,3}$, $G_{,3,3}$ $X_{2,9}$, $X_{3,9}$

Table 7. Characteristic Quantities of $D_{3,4}$, $E_{3,4}$, $G_{3,4}$, $D_{4,3}$

- Z-counting polynomial: $Q_G(X) = \sum_{k=0}^{m} p(G,k) X^k$

$$Q_G(X) = 113X^{12} - 4596X^{11} + 42006X^{10} - 155364X^{9} + 293637X^{8} - 320304X^{7} + 216232X^{6} - 93888X^{5} + 26613X^{4} - 4884X^{3} + 558X^{2} - 36X + 1$$

- Topological Index: $Z_G = \sum_{k=0}^{N/2} p(G,k) = 1158232$
- Characteristic polynomial: $P_G(X) = (-1)^N |A - XE| = \sum_{k=0}^{N} a_k X^{N-k}$

$$P_G(X) = X^{24} - 35X^{22} + 558X^{20} - 4916X^{18} + 27303X^{16} - 100056X^{14} + 245924X^{12} - 404088X^{10} + 435183X^{8} - 295684X^{6} + 118446X^{4} - 24660X^{2} + 2025$$

- $Z' = \sum_{k=0}^{N/2} (-1)^k a_{2k} = 1658880$
- $W = \sum_{j<k}^{N} D_{jk} = \sum_{k=1}^{d} k \ \ p_k = 768$

By inspecting the structure of these MLCFGs rather interesting relation came out. For example, $F_{3,5}$, $E_{3,5}$, $F_{5,3}$, and $E_{5,3}$ can be transformed into their corresponding H expression as follows. These graphs were not isomorphic each other, but their H expressions have some regularity (see Figure 10).

$$F_{3,5} = H(30, 5, -5),\ E_{3,5} = H(30, 7, -7),\ F_{5,3} = H(30, 9, -9),\ E_{5,3} = H(30, 11, -11) \qquad (12)$$

3.2. The Relatonship among the MLCFGs. Isomorphic relations among MLCFGs were also studied. For example,

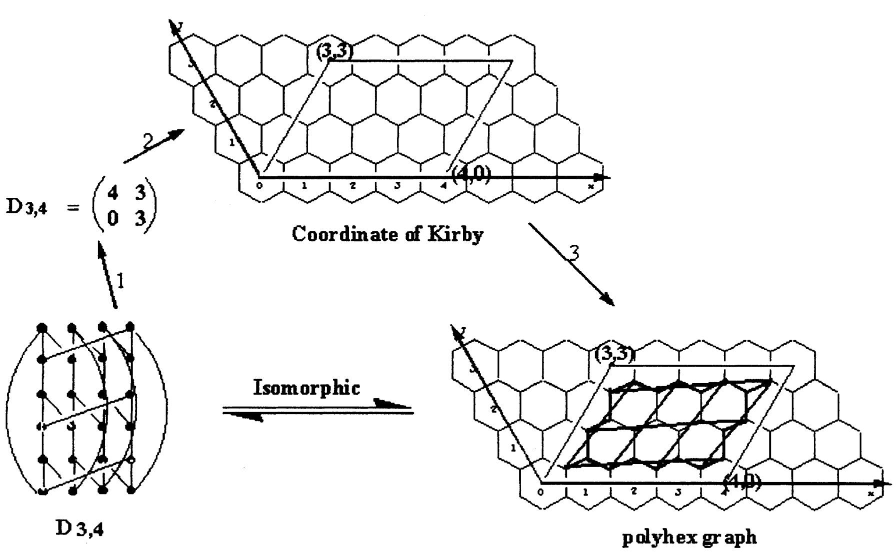

Figure 12. $D_{3,4}$ graph and the corresponding polyhex graph.

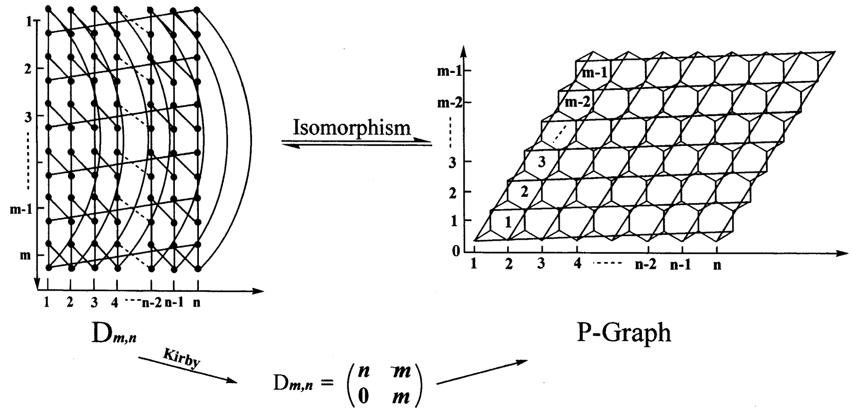

Figure 13. $D_{m,n}$ graph and the corresponding polyhex graph.

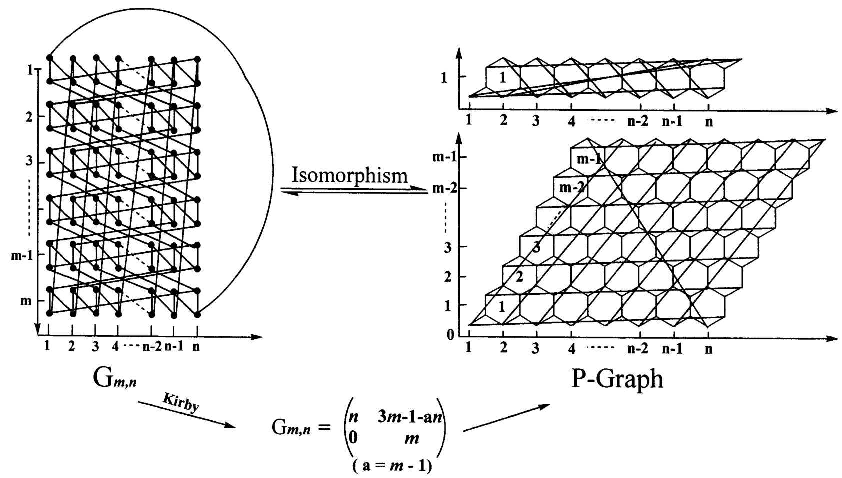

Figure 14. $G_{m,n}$ graph and the corresponding polyhex graph.

it is interesting to observe the isomorphism among $D_{3,4}$, $E_{3,4}$, $G_{3,4}$, and $D_{4,3}$ graphs though their construction schemes are all different (see Figure 11). Several of the characteristic quantities of $D_{3,4}$, $E_{3,4}$, $G_{3,4}$, and $D_{4,3}$ are also shown in Table 7.

For $D_{m,n}$, $G_{m,n}$, and $X_{m,n}$ families with lower members, it is interesting to observe the following isomorphic relations.

$$D_{m,2} = F_{m,2} = G_{m,2} \tag{13}$$

$$D_{2,n} = G_{2,n} \tag{14}$$

However for larger m and n, $D_{m,n}$ and $G_{m,n}$ families are not generally isomorphic to each other. As shown in Tables 4−6 lower members of D, G, and X families have isomorphic counterparts in MLCFG as exemplified in Figures 8 and 9.

3.3. Relationship between the MLCFG and Parallelogram-Shaped Polyhex Graphs. It was found that almost all the members of MLCFG can be systematically expressed in terms of the matrix by Kirby[4−6] as

$$E_{m,n} = \begin{pmatrix} n & m+1 \\ 0 & m \end{pmatrix}, F_{m,n} = \begin{pmatrix} n & 2m \\ 0 & m \end{pmatrix}, D_{m,n} \begin{pmatrix} n & m \\ 0 & m \end{pmatrix},$$
$$G_{m,n} = \begin{pmatrix} n & 3m-1-an \\ 0 & m \end{pmatrix} (a = m-1)$$

Namely, by using these matrices, every graph of the MLCFG (E, F, D, and G) can be transformed into their corresponding parallelogram-shaped P-graph mapped on the coordinate system of Kirby.[4−6] The polyhex graph included in the parallelogram is isomorphic to the corresponding MLCFG. For example, $D_{3,4}$ graph can be transformed into the corresponding polyhex graph (as shown in Figure 12).

In Figure 13 the relation between the $D_{m,n}$ and the corresponding polyhex graph is illustrated (see also Figure 8). Similar relation can be found for $G_{m,n}$ graphs as shown in Figures 9 and 14. On the other hand for $F_{m,n}$ and $X_{m,n}$ families no such regularity has even been discovered.

In this work we have calculated various characteristic quantities of a number of polyhex and torus graphs. As far as we have checked no isospectral pair of graphs nor "twin graph" were discovered.[25,26]

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