Multilayered Cyclic Fence Graphs: Novel Cubic Graphs Related to the Graphite Network

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Two series of multilayered cyclic fence grphs, $E_{m,n}$ and $F_{m,n}$, are proposed to be defined, both of which are composed of m $2n$-membered cycle graphs with periodic bridging and are all cubic and bipartite. Generalized Petersen graph, $P(n,\{j_k\})$, Hamiltonian wheel graph, $H(n,\{j_k\})$, and cyclic single-layered kagome graph, L_n, are also defined. Close relationships among these E, F, P, H, and L graphs are demonstrated, by which the exceedingly high symmetry of E and F families are discussed. Several members of E and F families were found to be isomorphic to the previously defined benzenoid torus networks which can span the infinitely large graphite network. By using the analytical expressions of the eigenvalues of $E_{m,n}$ and $F_{m,n}$ graphs the density of states of graphite can be simulated. Several members of E and F families were found to be the so-called integral graph with only integer eigenvalues.

INTRODUCTION

The present author has defined the series of cyclic fence graphs, E_n, by regular cyclization of the ethylene unit, or path graph, S_2, so that all the vertices have three neighbors.[1] This series of cubic graphs are all bipartite, i.e., without any odd-membered ring, and are found to be related to the family of polyhex graphs, i.e., composed of only hexagons, through the number of perfect matchings, or Kekulé number, $K(G)$. Besides this physicochemical feature, the cyclic fence graphs are also the target of graph-theoretical study in the sense that the spectra (the eigenvalues of the characteristic polynomial) of several members are found to be composed of only integers, and interesting recursive relations hold for the characteristic and matching polynomials.

Recently we have extended the concept of the fence graph to multilayered cyclic fence graphs (MLCFG) and found that all the members are isomorphic to the so-called "torus benzenoid graphs", which can be constructed by regular cyclization of polyhex graphs and have such a high symmetry that the electronic structure of these "torus molecules" rapidly converge to that of the graphite network.[2] Further, some members of MLCFG are found to be related to widely known graphs of graph-theoretical interest, such as the Hamiltonian and generalized Petersen graphs.[3,4]

In this paper some new findings of these MLCFGs will be presented with particular reference to their interesting mathematical features, such as their topological symmetry and eigenvalue distribution of the characteristic polynomial. The newly obtained 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.[5−12]

DEFINITIONS

Two families of multilayered cyclic fence graphs, $E_{m,n}$ and $F_{m,n}$, are defined as in Figures 1 and 2, respectively. Both of them are composed of m $2n$-membered cycle graphs (C_{2n}) with periodic bridging. Although there might be a possibility

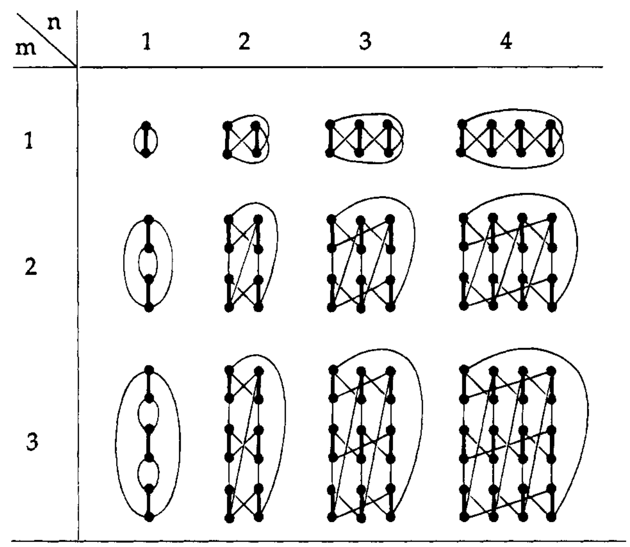

Figure 1. Lower members of $E_{m,n}$ family. Thick edges are just for clarifying the structure of the graph.

for the existence of other versions of multilayered cyclic fence graphs, in this paper we will mainly be concerned with these $E_{m,n}$ and $F_{m,n}$ graphs. As will later be shown that both of these two families of graphs can be mapped on a surface of a donut without edge crossing and thus can be called torus graphs with genus one.

For recognizing the symmetry of a given graph let us define two kinds of generalized Petersen graphs, $P(n,j)$ and $P(n,\{j_k\})$, (see Figure 3a),[13] and "Hamiltonian wheel graphs", $H(n,\{j_k\})$ (Figure 3b).

The skeleton of $P(n,j)$ and $P(n,\{j_k\})$ graphs is a cyclic comb graph[14] (marked with bold lines in Figure 3a) composed of a cycle graph C_n and n branches of unit length. $P(n,j)$ can be constructed by joining all the terminal vertices of the comb graph with their clockwise jth neighbors. The original Petersen graph can be denoted by $P(5,2)$, which is to have higher priority than $P(5,3)$. If this cyclic joining process is described by the repetition of $\{j_k\}$ steps with k = 1, 2, ⋯, p, the resultant graph is denoted by $P(n,\{j_k\})$ (see Figures 3−5), and called p-cyclic (generalized) Petersen graph.

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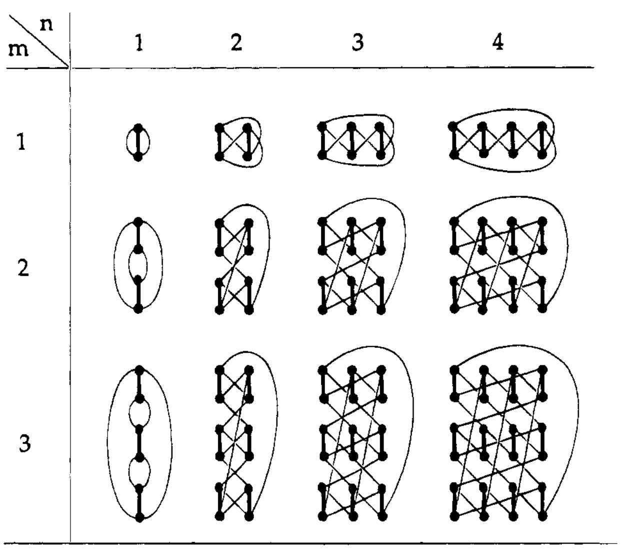

Figure 2. Lower members of $F_{m,n}$ family. Thick edges are just for clarifying the structure of the graph.

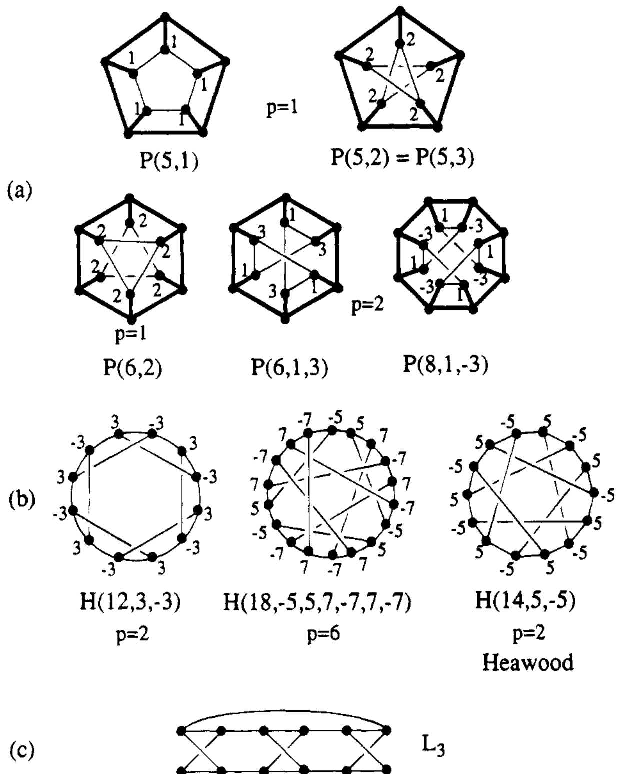

Figure 3. Definitions of (a) (p-cyclic) generalized Petersen graph, (b) Hamiltonian wheel graph, and (c) cyclic single-layered kagome graph.

It is obvious that

$$P(n,j,j) = P(n,j) \tag{1}$$

Further in the later discussions the following relations, though formal, will be shown to be effective for recognizing the isomorphicity of generalized Petersen graphs:

$$P(n,j,k) = P(n,k,j) \tag{2}$$

$$P(n,j,k) = P(n,-j,-k) \quad \text{and} \quad P(n,j) = P(n,-j) \tag{3}$$

$$P(n,j,k) = P(n,j \pm n,k) = P(n,j,k \pm n) \tag{4}$$

A (p-cyclic) Hamiltonian wheel graph, $H(n,\{j_k\})$ with $k = 1, 2, \cdots, p$, is constructed by p-periodic $\{j_k\}$-joining of n vertices of the cycle graph C_n as in the case of $P(n,\{j_k\})$ (see Figure 3b). In this notation the so-called Heawood graph,[4] or six-cage, is represented by $H(14,5,-5)$, which, however, is not directly related to either of the E or F graph.

Since the numbering scheme and principle are the same for H and P graphs, the same relations as eqs 1−4 for P graphs also hold for H graphs.

The cyclic single-layered kagome graph, L_n, is also defined as in Figure 3c. However, as will be shown below, L family is a member of either the E or F group.

Since $E_{m,n}$ and $F_{m,n}$ are bipartite and cubic (all vertices have three neighbors), only P and H graphs of these types will be discussed. The original Petersen graph is not bipartite and will not be treated here. It is to be noted here that such a one-cyclic Hamiltonian wheel graph, or $H(n,j)$, cannot be cubic. In the following discussion it will be shown that those E, F, P, H, and L graphs which are bipartite and cubic are closely related with each other.

ISOMORPHISM

Possibly due to their high symmetry the $E_{m,n}$ and $F_{m,n}$ families are redundant, especially for their lower members. Namely, the two series of graphs, $E_{1,n}$ and $F_{1,n}$, are isomorphic to each other and are nothing else but the cyclic fence graphs, E_n, which have already been defined by the present authors.[1] Similarly the two series of graphs, $E_{m,1}$ and $F_{m,1}$, are isomorphic to each other. Namely, we have,

$$E_{1,n} = F_{1,n} \quad (n \geq 1) \tag{5}$$

$$E_{m,1} = F_{m,1} \quad (m \geq 1) \tag{6}$$

Among these series of graphs one can immediately observe that

$$E_{1,4} = F_{1,4} = K_2 \times K_2 \times K_2 \quad \text{(cube graph)} \tag{7}$$

$$E_{1,2k} = F_{1,2k} = K_2 \times C_{2k} = P(2k,1) \quad (2k\text{-gonal prism}) \quad (k \geq 3) \tag{8}$$

and

$$F_{1,3} = K_{3,3} \text{ (complete bipartite graph).} \tag{9}$$

In a later discussion we will call $K_{3,3}$ as benzene torus graph.

It is easy to show that

$$E_{m,2} = F_{m,2} = L_m \ (m \geq 1) \tag{10}$$

However, for larger m and n, $E_{m,n}$ is not generally isomorphic to $E_{n,m}$, $F_{m,n}$, nor $F_{n,m}$.

Further, it is interesting to observe the following relations

$$E_{1,3} = F_{1,3}, E_{2,5} = F_{2,5} \tag{11}$$

or generally

$$E_{m,2m+1} = F_{m,2m+1} \ (m \geq 1) \tag{12}$$

However, many frustrating relations have been found as

$$F_{2,1} = F_{1,2}, F_{2,2} = F_{1,4}, F_{2,3} = F_{1,6}, \quad \text{but } F_{2,4} \neq F_{1,8} \tag{13}$$

$$F_{2,2} = F_{1,4}, F_{4,2} = F_{2,4}, \quad \text{but } F_{6,2} \neq F_{3,4} = E_{2,6} \qquad (14)$$

$$E_{3,2} \neq E_{2,3} = F_{3,2} \neq F_{2,3} \qquad (15)$$

$$E_{3,4} \neq E_{4,3} = F_{4,3} \neq F_{3,4} \qquad (16)$$

At this stage, except for eq 12, it is rather difficult to draw general rules for the isomorphicity between the pair of E and F graphs with the same set of m and n. Anyway as shown in Tables 1 and 2 (see also Figures 4 and 5) all the lower members of E and F families have isomorphic counterparts in the H family, while some selected members can be transformed into P forms. As has been stated and exemplified in Figures 4 and 5, almost all of E and F families were found to be isomorphic to torus networks derived from polyhex graphs (vide infra).

By noticing the zigzag Hamiltonian cycle any member of E family can be transformed into their corresponding H expression through the following relation (see Table 1)

$$E_{m,n} = H(2mn, 2m+1, -(2m+1)) \quad (m \geq 1) \qquad (17)$$

On the other hand, for F family there holds no such simple relation, but by trial-and-error method one can find all the corresponding H expressions (see Table 2). In some cases the H expression becomes rather complicated. For example, $F_{3,3}$ is isomorphic to $H(18,-5,5,7,-7,7,-7)$ (see Figures 3b and 5). In this case, since 18 peripheral dots of equal spacing on the circle are joined by six-cyclic "spoking", the resultant H graph has 3(=18/6) fold axis of rotation. Further, by taking into account the intrinsic properties of bridging (see eqs 2 and 3) one can say that the topological symmetry of $F_{3,3}$ graph is at least D_{3h}. In this sense the topological symmetry of the Heawood graph is at least D_{7h} (see Figure 3b).

TOPOLOGICAL SYMMETRY OF A GRAPH

As stated before, it is quite eqsy to find a zigzag Hamiltonian circuit for $E_{m,n}$, by use of which one can transform this graph into H form. Especially in the topological structure of $E_{2,n}$ graph one can observe two distinct $2n$-membered cycles (C_{2n}) and a set of $2n$ bridging edges between them. This leads us to an interesting property as

$$E_{2,n} = P(2n, 3, -5) \qquad (18)$$

Similarly for $F_{2,n}$ graphs one can obtain the following relation

$$F_{2,n} = P(2n, 5, -7) \qquad (19)$$

Application of these relations, together with the relations 1−4, to the lower members of E and F families gives us systematic understanding of the diversified results given in Tables 1 and 2. Namely, for E family we get[15]

$$E_{2,1} = P(2,3,-5) = P(2,1,1) = P(2,1) \qquad (20)$$

$$E_{2,2} = P(4,3,-5) = P(4,3,3) = P(4,3) = P(4,1) \qquad (21)$$

$$E_{2,3} = P(6,3,-5) = P(6,3,1) = P(6,1,3) \qquad (22)$$

$$E_{2,4} = P(8,3,-5) = P(8,3,3) = P(8,3) \qquad (23)$$

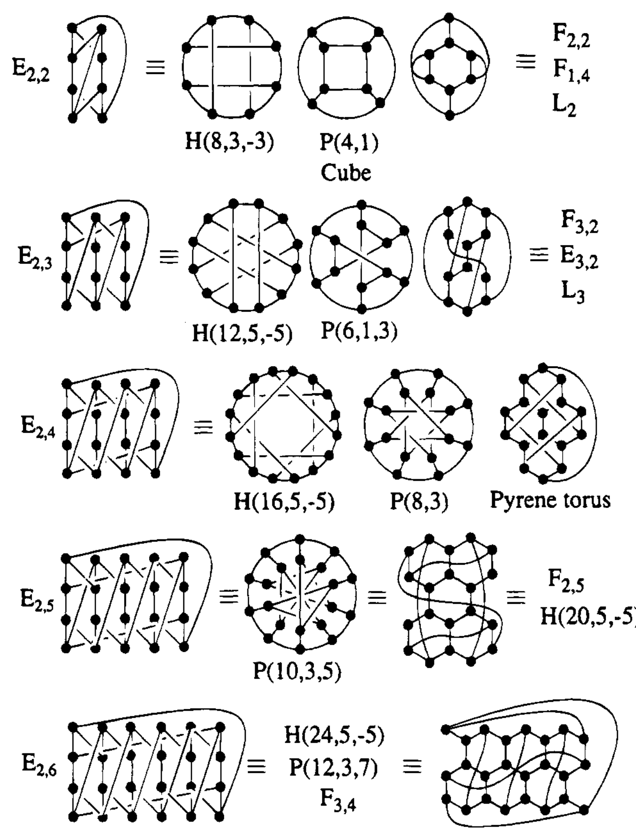

Figure 4. Isomorphism of $E_{m,n}$ graphs.

$$E_{2,5} = P(10,3,-5) = P(10,3,5). \qquad (24)$$

For F family similar results can be obtained as

$$F_{2,1} = P(2,5,-7) = P(2,1,1) = P(2,1) \qquad (25)$$

$$F_{2,2} = P(4,5,-7) = P(4,1,1) = P(4,1) \qquad (26)$$

$$F_{2,3} = P(6,5,-7) = P(6,5,5) = P(6,5) = P(6,1) \qquad (27)$$

$$F_{2,4} = P(8,5,-7) = P(8,5,1) = P(8,1,5) \qquad (28)$$

$$F_{2,5} = P(10,5,-7) = P(10,5,3) = P(10,3,5) \qquad (29)$$

Although the H expressions for E family are simple and systematic, those for F family are difficult to explain except for the lowest members (with m or n being 2) as has already been pointed out. For example, the H expressions for $F_{m,6}$ are generally rather complicated, and the topological symmetry of these graphs seems to be lower compared to other members of similar size, e.g., as low as D_{4h} ($F_{2,6}$), D_{6h} ($F_{3,6}$), D_{4h} ($F_{4,6}$), etc.

However, by inspecting the topological structure of these MLCFGs rather interesting features came out. For example, $F_{2,6}$ graph is found to be isomorphic not only to the so-called coronene torus which is derived from the cyclic wrapping of the coronene skeleton (see Figure 6) but also to a variety of graphs ranging from D_{3h} to D_{12h} as shown in Figure 7. That $F_{2,6}$ is a mathematically defined torus can be understood from Figure 7f, which apparently can be mapped on a surface of a donut. Similarly all the members of E and F families are shown to be tori.[16] However, among them all the $E_{1,2m}$ $= F_{1,2m}$ graphs are planar.

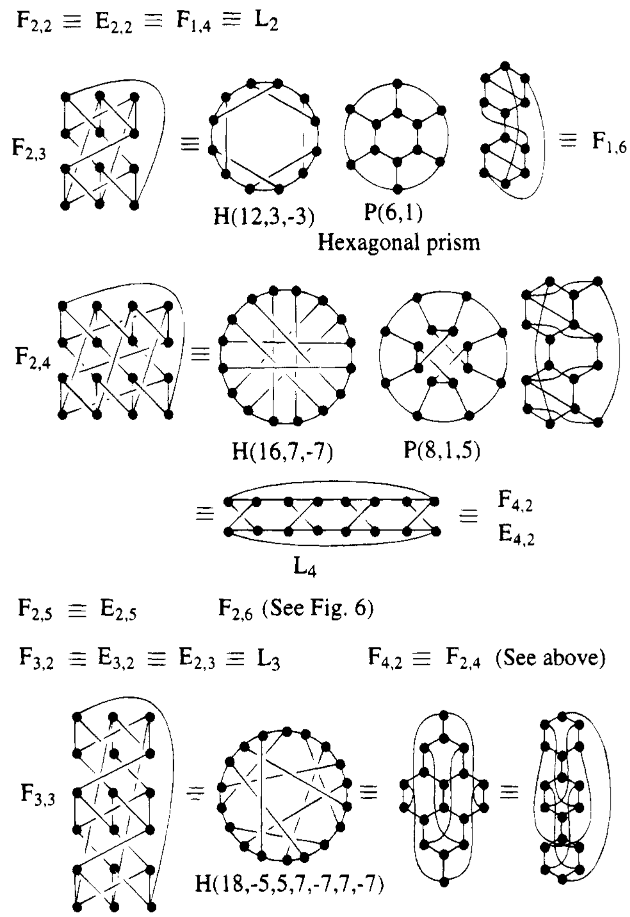

Figure 5. Isomorphism of $F_{m,n}$ graphs.

Table 1. Isomorphism and Various Properties of $E_{m,n}$ Family[a]

	m			
n	1	2	3	4
1	H(2,1)* x	H(4,1−1) P(2,1)	H(6,1−1) x	H(8,1−1) x
2	H(4,1,−1)* P(2,1)*	H(8,3,−3)* P(4,1)*	H(12,5,−5) P(6,1,3)	H(16,7,−7) P(8,1,−3)
3	H(6,3)* x	H(12,5,−5) P(6,1,3)	H(18,7,−7) x	H(24,9,−9)
4	H(8,3,−3)* P(4,1)*	H(16,5,−5) P(8,3)	H(24,7,−7)	H(32,9,−9)
5	H(10,3,−3) x	H(20,5,−5) P(10,3,5)	H(30,7,−7) x	H(40,9,−9)
6	H(12,3,−3)* P(6,1)*	H(24,5,−5) P(12,3,−5)	H(36,7,−7)	H(48,9,−9)
7	H(14,3,−3) x	H(28,5,−5) P(14,3,−5)	H(42,7,−7) x	H(56,9,−9)
8	H(16,3,−3) P(8,1)	H(32,5,−5) P(16,3,−5)	H(48,7,−7)	H(64,9,−9)
9	H(18,3,−3) x	H(36,5,−5) P(18,3,−5)	H(54,7,−7) x	H(72,9,−9)
10	H(20,3,−3) P(10,1)	H(40,5,−5) P(20,3,−5)	H(60,7,−7)	H(80,9,−9)

[a] Underlined, vertex and edge topicities are both unity; H, Hamiltonian wheel graph; P, generalized Petersen graph; x, no corresponding Petersen graph; *, integral graph.

The coronene torus ($F_{2,6}$) and pyrene torus ($E_{2,4}$, see Figure 4) were found to have exceeding high symmetry so that all edges and vertices are respectively equivalent.[2] In graph-theoretical terminology, its edge and vertex topicities are all unity.[17] Besides $F_{2,6}$ several other members of E and F families such as $E_{2,4}$ were found to have this novel property. In Tables 1 and 2 those graphs are underlined whose edge

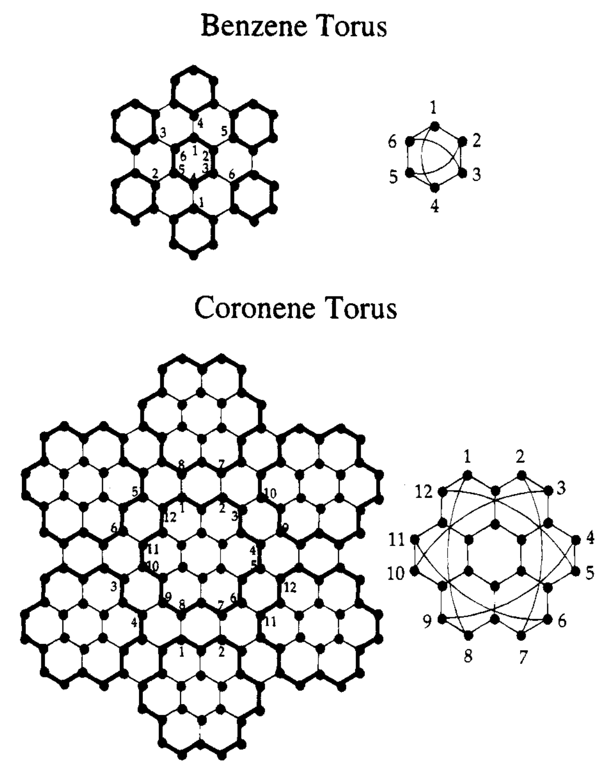

Figure 6. Mapping of benzene ($E_{1,3} = F_{1,3}$) and coronene ($F_{2,6}$) tori on the graphite network.

and vertex topicities are both unity.

SPECTRA OF GRAPHS

From algebraic standpoint the symmetry of a given graph can be checked by the distribution of eigenvalues or spectra in mathematical terminology.[14,18] Actually the characteristic polynomial, $P_G(x) = (-1)^N \det(\mathbf{A} - x\mathbf{E})$, of E and F families is generally highly factorable, where $\mathbf{A}$ and $\mathbf{E}$ are, respectively, the adjacency and unit matrices. If one carefully observes its cyclic structure, the $P_G(x)$ of $F_{m,n}$ can be factored out as

$$P_{F_{m,n}}(x) = \prod_{j=1}^{n}\prod_{k=1}^{m}\begin{vmatrix} -x & 1 + a + a^* b^* \\ 1 + a^* + ab & -x \end{vmatrix} = \prod_{j=1}^{n}\prod_{k=1}^{m}\left\{x^2 - \left[3 + 2\cos\frac{2j\pi}{n} + 2\cos\left(\frac{2j\pi}{n} + \frac{2k\pi}{m}\right) + 2\cos\left(\frac{4j\pi}{n} + \frac{2k\pi}{m}\right)\right]\right\} \quad (30)$$

with

$$a = \exp\left(\frac{2j\pi}{n}i\right), \qquad b = \exp\left(\frac{2k\pi}{m}i\right)$$

A detailed recipe for this factorization has been described elsewhere.[19-21]

Since an $E_{m,n}$ graph is represented by a two-cyclic H graph, its characteristic polynomial can also be factored out into the product of mn determinants of 2×2. Namely,

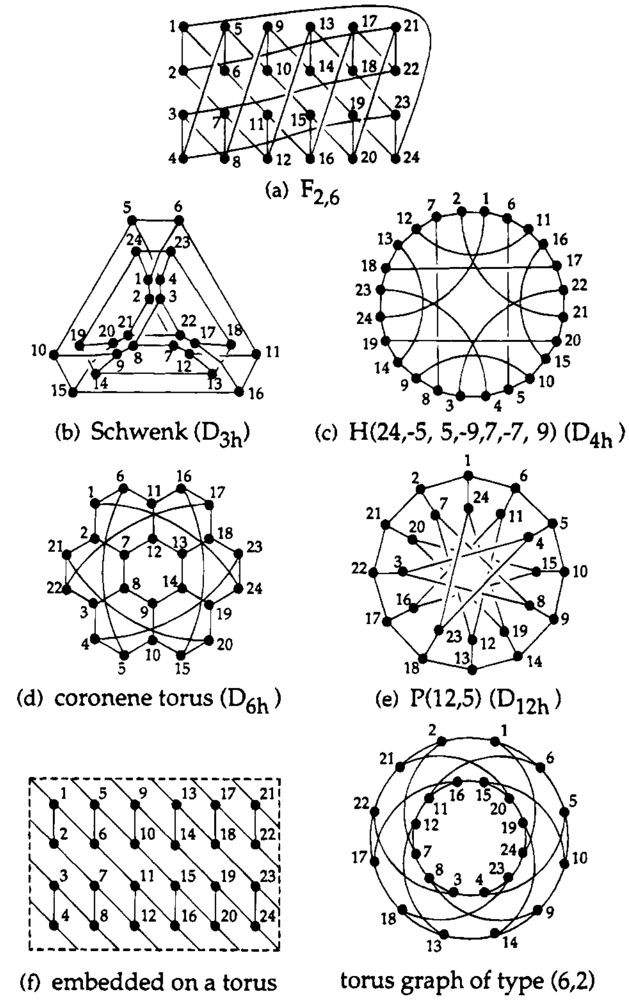

Figure 7. Isomorphism of $F_{2,6}$ graph.

$$P_{E_{m,n}}(x) = \prod_{k=1}^{mn} \begin{vmatrix} -x & 1 + a^* + a^m \\ 1 + a + a^{*m} & -x \end{vmatrix} = \prod_{k=1}^{mn} \left\{ x^2 - \left[3 + 2\cos\frac{2k\pi}{mn} + 2\cos\frac{2k\pi}{n} + 2\cos\left(\frac{2(m+1)k\pi}{mn}\right) \right] \right\} \quad (31)$$

with

$$a = \exp\left(\frac{2k\pi}{mn} i\right)$$

Thus all the spectra of MLCFGs have been analytically solved.

According to the established Hückel molecular orbital theory the charge density on each carbon atom (vertex) of an alternant hydrocarbon molecule (bipartite graph) is all unity.[22,23] Further, one can calculate the bond orders for all the edges of a given graph by using the wave functions (eigenvectors of $\mathbf{A} - x\mathbf{E}$ matrix). The edge topicity of a given graph can be judged from the set of bond orders, although the vertex topicity cannot be deduced from the calculated charge density in this case.

Thus by checking their spectral distribution, highly symmetrical members were sorted out including $E_{2,4}$ and $F_{2,6}$ introduced in the preceding section.

Table 2. Isomorphism and Various Properties of $F_{m,n}$ Family[a]

	m		
n	2	3	4
2	$F_{1,4}$ $\underline{H(8,3,-3)^*}$ $\underline{P(4,1)^*}$	$E_{2,3}$ $H(12,5,-5)$ $P(6,1,3)$	$F_{2,4}$ $H(16,7,-7)$ $P(8,1,-3)$
3	$F_{1,6}$ $H(12,3,-3)^*$ $P(6,1)^*$	 $\underline{H(18,-5,5,7,-7,7,-7)}$ x	$E_{4,3}$ $H(24,9,-9)$ x
4	$F_{4,2}$ $H(16,7,-7)$ $P(8,1-3)$	$E_{2,6}$ $H(24,5,-5)$ $P(12,3,-5)$	 $H(32,5,-5,13,-13)$ $P(16,3,7)$
5	$E_{2,5}$ $H(20,5,-5)$ $P(10,3,5)$	 $H(30,5,-5)$ x	 $H(40,7,-7)$ x
6	 $\underline{H(24,-5,5-9,7,-7,9)^*}$ $\underline{P(12,5)^*}$	 $H(36,-5,5,7,-7,7,-7)$ $P(18,3,3,3,-7,-5,5)$	$F_{2,12}$ $H(48,-7,7,-7,7,$ $-7,7,9,-9)$ $P(24,5,-7)$
7	 $H(28,7,-7)$ $P(14,5,7)$	$E_{3,7}$ $H(42,7,-7)$ x	 $H(56,7,-7)$ x
8	$H(32,-11,11,7,-7)$ $P(16,5,-7)$	$H(48,19,-19)$ $P(24,7,-9)$	$H(64,-15,15,17,-17)$ $P(32,3,7,3,-9)$
9	 $H(36,9,-9)$ $P(18,5,-7)$	 $H(54,11,-11,11,-11,$ $-13,13)$ x	$E_{4,9}$ $H(72,9,-9)$ x
10	$H(40,11,-11,-13,13)$ $P(20,5,-7)$	$H(60,17,-17)$ $P(30,9,-11)$	$H(80,-11,11,13,-13)$ $P(40,9,-11)$

[a] See Table 1 for $F_{1,n}$ and $F_{m,1}$. Underlined, vertex and edge topicities are both unity; H, Hamiltonian wheel graph; P, generalized Petersen graph; x, no corresopnding Petersen graph; *, integral graph.

Interestingly enough, the eigenvalues of $F_{2,6}$ are all integers, so that $F_{2,6}$ may be called an integral graph.[24] One of its isomorphic drawings, Figure 7b, was drawn by Schwenk who proved that there exist only eight bipartite cubic integral graphs,[24] half of which were found to belong to the F family. In Tables 1 and 2 these integral graphs are asterisked.

CONVERGENCE TO GRAPHITE NETWORK

One can consider a series of torus networks of regular hexagonal structure extending from benzene and coronene tori toward the infinitely large graphite network as seen in Figure 8. This series of graphs is isomorphic to our $F_{m,3m}$ graphs, whose spectra can be obtained analytically. The spectral distribution of fairly large networks with about 50 000 carbon atoms of this series of graphs was calculated as shown in Figure 9, which reproduces exactly the density of states of graphite. Thus we can safely use this series of tori or $F_{m,3m}$ networks for obtaining detailed information on the electronic structure of graphite and related problems, such as the growing process of graphite and chemical adsorption reaction onto the surface of graphite.[2] Similarly the series of $E_{m,m+2}$ (see Figure 8) and other series of graphs were also found to converge to graphite. Although the speed of convergence of the density of states is rather low, we have already shown that other electronic properties, such as the energy per π-electron, bond order, etc., were found to converge to the values for the infinitely large graphite network.[2,24] Studies are being in progress for clarifying the mathematical structure of this interesting series of graphs.

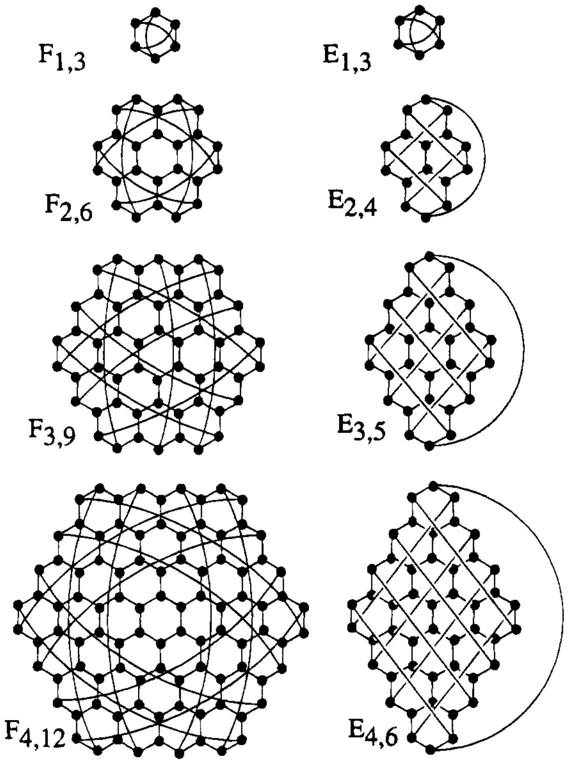

Figure 8. Two series of multi-layered cyclic fence graphs, $F_{m,3m}$ and $E_{m,m+2}$ converging toward the graphite network.

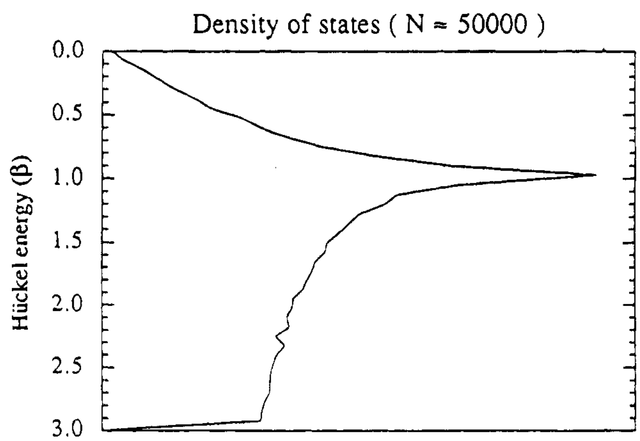

Figure 9. Profile of the spectral distribution of large $F_{m,3m}$ graph ($3m \approx 50\,000$) which rigorously approaches the density of states of the electronic structure of graphite. The lower half part (filled band) is shown.

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REFERENCES AND NOTES

(1) Hosoya, H.; Harary, F. On the Matching Properties of Three Fence Graphs. *J. Math. Chem.* **1993**, *12*, 211−218.

(2) Hosoya, H.; Tsukano, Y.; Ohuchi, M.; Nakada, K. 2-Dimensional Torus Benzenoids Whose Electronic State Rapidly Coverges to Graphite. In *Computer Aided Innovation of New Materials II*; Doyama, M., Kihara, J., Tanaka, M., Yamamoto, R., Eds.; Elsevier: Amsterdam, 1993; pp 155−158.

(3) Exoo, G.; Harary, F.; Kabell, J. The Crossing Numbers of Some Generalized Petersen Graphs. *Math. Scand.* **1981**, *48*, 184−188.

(4) Harary, F. *Graph Theory*; Addison-Wesley, Reading, MA, **1969**.

(5) Balaban, A. T.; Farcasiu, D.; Banica, R. Chemical Graphs. II. Graphs of Multiple 1,2-Shifts in Carbonium Ions and Related Systems. *Rev. Roum. Chim.* **1966**, *11*, 1205−1227, and the subsequent series of papers.

(6) Muetterties, E. L. Topological Representation of Stereoisomerism. I. Polytopal Rearrangements. *J. Am. Chem. Soc.* **1969**, *91*, 1636−1643.

(7) Clark, M. J.; Kettle, S. F. A. Incidence and Distance Matrices. *Inorg.* Chim. *Acta* **1975**, *14*, 201−205.

(8) Dugundji, J.; Gillespie, P.; Marquarding, D.; Ugi, I.; Ramirez, F. Matric Spaces and Graphs Representing the Logical Structure of Chemistry. In *Chemical Applications of Graph Theory*; Balaban, A. T., Ed.; Academic Press: London, 1976.

(9) Gielen, M. Applications of Graph Theory to Organometallic Chemistry. In *Chemical Applications of Graph Theory*; Balaban, A. T., Ed.; Academic Press: London, 1976.

(10) Randić, M. On Discerning Symmetry Properties of Graphs. *Chem. Phys. Lett.* **1976**, *42*, 283−287.

(11) Balasubramanian, K. Applications of Combinatorics and Graph Theory to Spectroscopy and Quantum Chemistry. *Chem. Rev.* **1985**, *85*, 599−618.

(12) Sato, M. Hamiltonian Graph Representation of Zeolite Frameworks and Si, Al Ordering in the Framework. *J. Math. Chem.* **1991**, *7*, 341−352.

(13) In ref 3 $P(n,\{j_k\})$ is not defined.

(14) Hosoya, H. Factorization and Recursion Relations of the Matching and Characteristic Polynomials of Periodic Polymer Networks. *J. Math. Chem.* **1991**, *7*, 289−305.

(15) Instead of $P(2,1,-1)$ the notation $P(2,1)$ may be used under such condition that only cubic graphs are concerned.

(16) Dr. J.-I. Aihara of Shizuoka University kindly pointed out that E and F can be mapped on a surface of a donut.

(17) Walba, D. M.; Harary, F. Topicity of Vertices and Edges in the Möbius Ladders: A Topological Result with Chemical Implications. *Tetrahedron Lett.* **1988**, *29*, 731−734.

(18) Cvetković, D.; Doob, M.; Sachs, H. *Spectra of Graphs. Theory and Applications*; Academic Press, Berlin, 1979.

(19) Hosoya, H.; Aida, M.; Kumagai, R.; Watanabe, K. Analysis of the π-Electronic Structure of Infinitely Large Networks. I. Some Remarks on the Characteristic Polynomial and Density of States of Large Polycyclic Aromatic Hydrocarbons. *J. Comput. Chem.* **1987**, *4*, 358−366.

(20) Unpublished but see, also: Hosoya, H. Electronic Structure of Benzenoid Torus Networks Rapidly Converging to Graphite. *Abstract of The 2nd Japan-China Synposium on Theoretical Chemistry*; Kyoto, Japan, 1992; pp 81−82. Hosoya, H. Geometrical Symmetry and Topological Symmetry. *Abstract of 1st Congress of the International Society for Theoretical Chemiscal Physics*; Girona, Spain, 1993.

(21) Liu, J.; Shao, Y. H.; Jiang, Y. S. Exact Solution of Graph Spectrum of C_{60}. *Chem. Phys. Lett.* **1993**, *210*, 149−152.

(22) Coulson, C. A.; Rushbrooke, S. The Method of Molecular Orbitals. *Proc. Cambridge Phil. Soc.* **1940**, *36*, 193−200.

(23) Trinajstić, N. *Chemical Graph Theory*; CRC Press: Boca Raton, FL, 1983.

(24) Schwenk, A. J. *Exactly Thirteen Connected Cubic Graphs Have Integral Spectra.* Lecture Notes in Mathematics (Theory and Applications of Graphs); Alavi, Y., Lick, D. R. Eds.; Springer: 1978; Vol. 642, pp 516−533.

(25) Tsukano, Y. Master Thesis, Ochanomizu University, 1994.

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