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Supersymmetry of Hexabenzocoronene Torus*

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Key words Hexabenzocoronene torus (HBCT) is a hypothetical torus-shaped network derived by properly connecting the nine pairs of peripheral carbon atoms of the hexabenzocoronene skeleton. The π -electronic structure of this hypothetical conjugated carbon network has an exceedingly high symmetry (supersymmetry) and is closely related to that of the graphite network. By using the group-theoretic technique developed by the authors it is shown that this 42×42 secular determinant of HBCT can be factorized into the product of 21 quadratic equations. A number of interesting mathematical properties of the supersymmetry of HBCT are introduced.

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INTRODUCTION

The discovery of fullerenes¹ and nanotubes² triggered vigorous study of the mathematical and electronic structure of torus networks under various names, *e.g.*, toronoid, torene, *etc.*^{3–10} Most of the research groups were concerned with the 3-dimensional torus-shaped carbon networks of genus 1. On the other hand, our group discovered that if one constructs several series of hypothetical benzenoid torus networks (see Figure 1) by properly joining all the distant pairs of peripheral carbon atoms of several types of 2-dimensional polycyclic aromatic hydrocarbons, *i.e.*, coronene (a), pyrene (b), and hexabenzocoronene (c), their π -electronic structures rapidly converge to that of the infinitely large graphite network.¹¹

Namely, relatively small torus networks of these series with a few hundred carbon atoms were shown to be used for model systems of the π -electronic structure of graphite, whereas more than a hundred thousand carbon atoms are necessary for their parent hydrocarbon molecules to gain the graphite property.¹² Although the tori discussed in this paper seem to be rather different in a chemical sense from what are treated by other research groups, they are found to belong to the non-planar toroidal hydrocarbons according to the classification proposed by Trinajstić.¹³

Recently Stewart found that by using our tori as unit cells new mathematics of symmetry groups of a third type (between point groups and space groups) can be

* Dedicated to Professor Nenad Trinajstić on the occasion of his 65th birthday.

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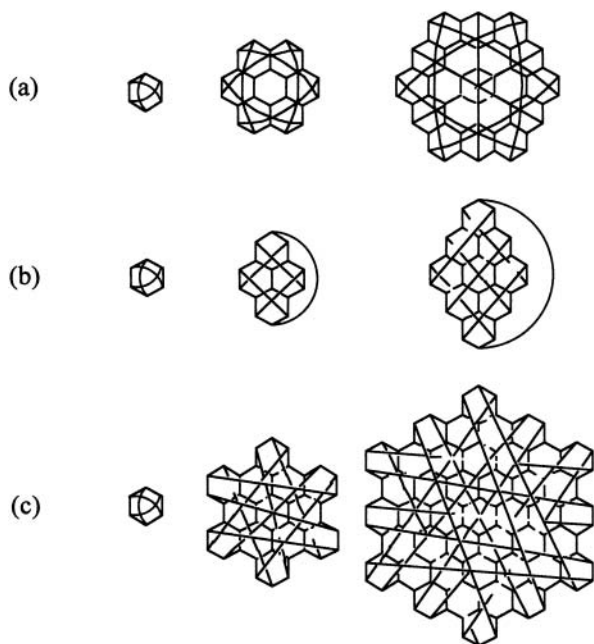


Figure 1. Three series of hypothetical benzenoid torus networks. (a) coronene, (b) pyrene, and (c) hexabenzocoronene.

constructed for discussing the properties of infinitely large lattices such as graphite.¹⁴

On the other hand, Aihara *et al.* found that the hypothetical 54-carbon network (see Figure 1a) of the next higher member of the coronene torus, or supercoronene torus, can be used as the reference structure for the π -electronic properties of the infinitely large graphite and graphitic tubulene networks.¹⁵

Besides these physico-chemical features the series of the torus networks in Figure 1 were found to have interesting graph-theoretical characteristics, *e.g.*, exceedingly high symmetrical properties and isomorphic relations. A number of other torus series were found and their topological symmetry was extensively studied by our group.¹⁶ Both the series of (a) and (b) torus networks were found to be isomorphic to generalized Petersen and Heawood graphs¹⁷ and multilayered cyclic fence graphs (MLCFGs).^{18–20} Since most of the results of hexabenzocoronene torus (HBCT) graphs, (c), have not been published yet, their interesting mathematical properties are introduced in this paper with particular reference to its highly symmetrical properties.

HEXABENZOCORONENE TORUS

Hexabenzocoronene (HBC), or *hexa-peri*-benzocoronene, existing in yellow crystalline state is noted for its extreme stability. Namely, it does not dissolve into concentrated sulfuric acid, and its melting point could not be determined because the melting-point tube melted long before the hydrocarbon.²¹ According to Clar it belongs to the most stable group of aromatic hydrocarbons called

»fully benzenoids« whose ground states are best described by the following structural formula, a symbol mark of his aromatic sextet theory, composed of only (resonant) sextets (depicted by circles) and no isolated double bond.²²



Later graph-theoretical basis and interpretation for the empirically derived Clar's aromatic-sextet theory were given by our group.^{23–25} In this sense HBC and HBCT have an important role in the discussion of the π -electronic stability of polycyclic aromatic hydrocarbons and graphite network.

The idea of the construction of the series of torus graphs in Figure 1 naïvely comes from the problem of periodically homogeneous tiling of the graphite network. The π -electronic structure of graphite in the HMO approximation can easily be factored out into the product of 2×2 determinants.²⁶ In this case the π -electronic system of ethylene is the tiling unit to span the entire network. Similarly a number of polycyclic aromatic hydrocarbon molecules, such as benzene, naphthalene, pyrene, coronene, *etc.* can be the tiling unit.^{16,27}

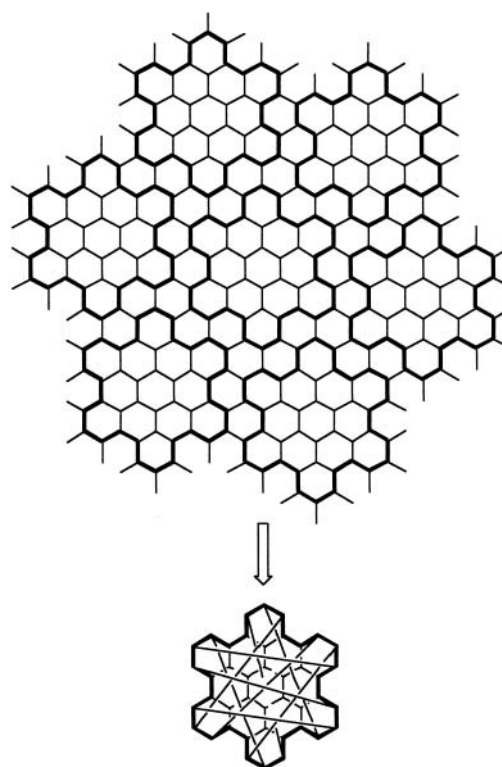


Figure 2. Criterion for constructing the torus of hexabenzocoronene from the tiling of the graphite network.

As shown in Figure 2, HBC and its higher members are also found to have this property. The mode of joining the distant pairs of the peripheral carbon atoms to yield a »torus« structure is uniquely determined so that the interunit $i-j'$ bond is cut and rejoined to form $i-j$ (bridging) bond within the unit.

Then there arises a problem. Does the resultant network really have the property of a mathematically defined torus? The answer is »Yes« as will be shown later in this paper.²⁸ Further, it was found that our HBCT can be identified by a triplet of integers proposed by Klein in his generalized expression for toroidal benzenoid networks.²⁹

C₆ ROTATIONAL SYMMETRY

The six-fold rotational symmetry of the structure of HBCT is easily seen as in Figure 3. Six benzyl radicals are joined together through short and long (bridging) bonds to form the network of HBCT. Note that there is no difference in strength among all the bonds. In this special case each benzyl radical unit is connected to all other five units.

Then by using the recipe³⁰ for the graph with rotational symmetry in a topological sense one can factorize the Hückel determinant of HBCT into the product of the six 7×7 determinants of the cyclic monomer of benzyl radical, which can be obtained by adding the contribution of bridging to the respectively corresponding element in the determinant of the cyclic monomer unit.

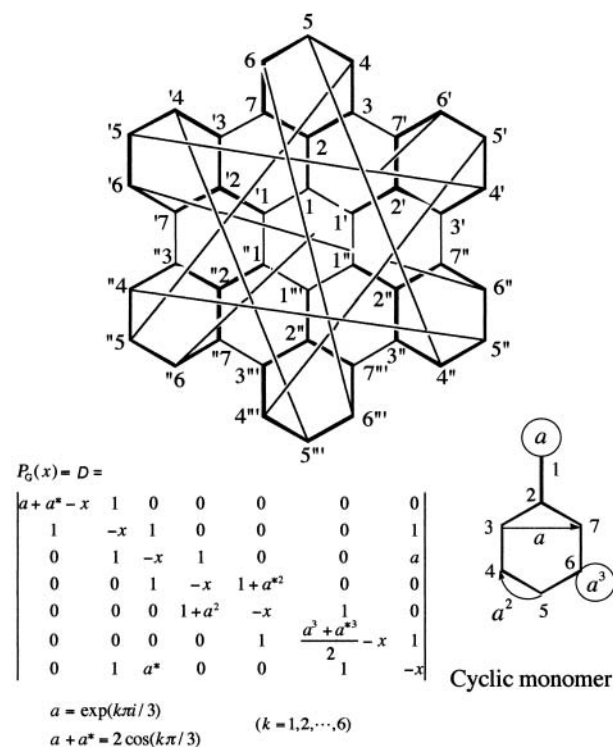


Figure 3. Factorization of the secular determinant of HBCT into that of the benzyl radical-shaped cyclic monomer.

Namely, if the r -th atom in a tiling unit is joined with the s -th atom in the clockwise j -th unit, the term a^j ($a = \exp(2k\pi i/6)$, ($k = 1, \dots, 6$)) is added to the (r, s) element of the secular determinant of the parent skeleton of the cyclic monomer, while the complex conjugate a^{*j} to the (s, r) element to make the determinant Hermitian.

The resultant secular determinant D and modified structural formula of the cyclic monomer of benzyl radical are shown in Figure 3, where an arrows and loops depict the bridging interactions.

By expanding D for the respective values of $k = 1 \sim 6$ one gets

$$D = \begin{cases} x A & k = 1, 2, 4, 5 \\ (x + 3) A & k = 3 \\ (x - 3) A & k = 6 \end{cases} \quad (1)$$

with

$$A = x^6 - 9x^4 + 21x^2 - 14 = (x^2 - 2)(x^4 - 7x^2 + 7) \quad (2)$$

This means that the 42 eigenvalues of HBCT are highly degenerate. There are six sets of 6-fold degeneracy, a set of quadruplet NBMO's, and a non-degenerate pair of the lowest and highest orbitals ($x = \pm 3$), the last of which necessarily come from a cubic graph. In fact the degrees of all the vertices of HBCT and other tori are three.

It is remarkable that the eigenvalues of HBCT can be solved by at most quadratic equations, revealing the existence of some hidden higher symmetry. Actually, as seen in Figure 4 HBCT is more highly degenerate than the parent HBC, which, however, has a pair of 6-fold degenerate levels. This unusually high degeneracy of HBC might be accidental, possibly because their values are ± 1 .

A similar relation is also observed in the eigenvalues of the pair of coronene and its torus. The 24 eigenvalues of the coronene torus are distributed as $(\pm 3, \pm 2^6, \pm 1^3, 0^4)$, while the parent coronene has a pair of triply degenerate

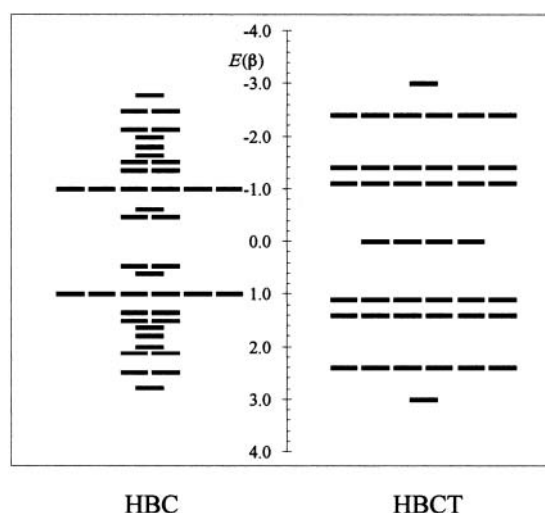


Figure 4. Hückel MO energy level diagrams of the HBC and its torus, HBCT.

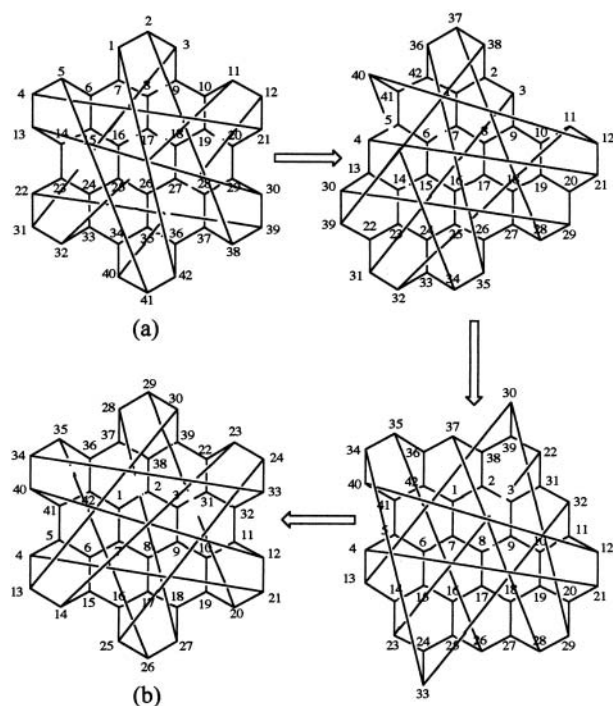


Figure 5. Edge-transitive property of HBCT. Compare the relative sites in (a) and (b) of the seven benzene rings which are located at the aromatic sextets in the Clar pattern of the parent HBC.

erate (± 1), six doubly degenerate, and six non-degenerate orbitals. In graph theory this graph is known to be one of the eight bipartite »integer graphs« discovered by Schwenk.³¹ The only triply degenerate pair of coronene eigenvalues is also thought to be accidental, because their values are again ± 1 .

Anyway the unusually high symmetry of these torus graphs is possibly due to the lack of a peripheral region as in the graphite network. However, just the lack of peripheral region does not necessarily explain the abnormally high symmetry of HBCT, since many other benzenoid torus networks were found to have lower symmetry than HBCT.¹⁶

The bond orders of all the bonds in HBCT were calculated to have the same value of 0.5126. Namely, this network is not only vertex-transitive but also edge-transitive.³² In other words both the topologies of vertex and edge of HBCT are unity.³³

The edge-transitive property of HBCT can be demonstrated as in Figure 5, where the mapping (a) is transformed into (b) step-by-step by changing the geometrical shape of the graph constructed as if from elastic strings.

C₇ ROTATIONAL SYMMETRY

Close examination of Figure 5 reveals that all the seven »Clar's aromatic sextets« of the HBC skeleton are circularly changing their positions one by one according to some rule. Thus the aromatic sextet pattern of HBC pro-

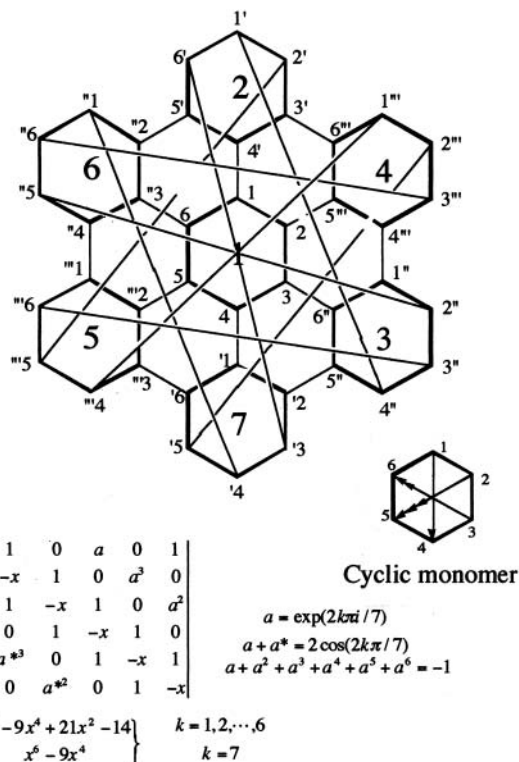


Figure 6. Factorization of the secular determinant of HBCT into that of the benzene-shaped cyclic monomer. Compare with Figure 3.

posed by Clar^{22,25} gave us a hint to disclose the hidden 7-fold symmetry of the HBCT network. See Figure 6 and trace the cyclic structure of HBCT where the numbered seven benzene rings located just on the aromatic sextets of HBC are connected to form a big ring and span the whole skeleton.

In the cyclic monomer of this network the number of arrowheads indicates the difference between the numbers (or the count of the steps) assigned to the cyclic monomers which are connected by the bridging bonds. It is to be noted here that a cyclic monomer, or the aromatic sextet of HBC, is connected to all six other members through the bridging bonds forming the skeletal structure of the HBCT network.

The 6×6 determinant of the cyclic monomer of HBCT were found to be simpler than for the case of the 6-fold symmetry. Namely, all the different k values except for $k = 7$ yield the same polynomial D of order six, clearly showing the essentially 6-fold degeneracy of the eigenvalues of HBCT.

HAMILTONIAN CYCLE AND HEAWOOD GRAPH

In the study of multilayered cyclic fence graphs a number of benzenoid torus graphs were found to have a Hamiltonian cycle of high symmetry.^{18,20,27} After trial and error search on the HBCT network we found a Hamiltonian cycle as shown in Figure 7.

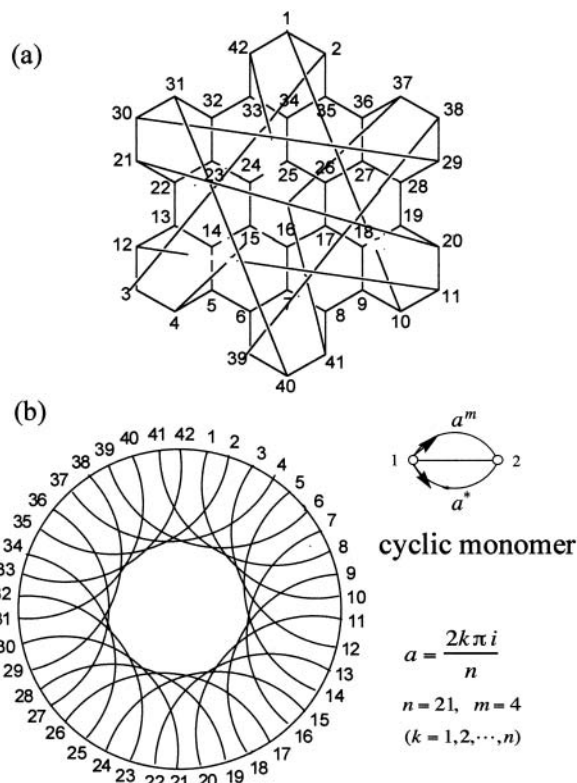


Figure 7. A Hamiltonian cycle (a) and a circular diagram, or generalized Heawood graph, (b) of HBCT.

Namely, by tracing the zigzag path along the numbers from 1 to 42 and back to 1 as shown in (a) a Hamiltonian cycle is obtained, with which one can redraw the network of HBCT into a circular diagram (b) of 21-fold rotational symmetry in a topological sense. It can be said that this graph belongs to D_{21h} point group. Each odd numbered vertex is bridged to the clockwise ninth vertex, while each even numbered vertex is bridged to the counterclockwise ninth vertex. Then according to our definition¹⁸ Figure 7b is a generalized Heawood graph, $H(42, 9, -9)$, whose topological structure can be reduced to the cyclic monomer consisting of only two vertices. Vertex 1 is bonded triply to vertex 2, *i.e.*, of the same, fourth next, and minus first next cyclic monomers. Then the secular determinant of this cyclic monomer is obtained as follows:

$$\begin{vmatrix} -x & 1+a^m+a^* \\ 1+a^{*m}+a & -x \end{vmatrix}$$

$$= x^2 - \left\{ 3 + 2\cos\frac{2k\pi}{n} + 2\cos\frac{2km\pi}{n} + 2\cos\frac{2k(m+1)\pi}{n} \right\} \quad (3)$$

$$a = \frac{2k\pi i}{n} \quad (k = 1, 2, \dots, n)$$

with $n = 21$ and $m = 4$. The 42 eigenvalues of HBCT are given by

$$x = \pm \sqrt{3 + 2\cos\frac{2k\pi}{21} + 2\cos\frac{8k\pi}{21} + 2\cos\frac{10k\pi}{21}}$$

$$(k = 1, 2, \dots, 21) \quad (4)$$

By putting 21 different integers into k one gets

$$x = \begin{cases} 0 & k = 7, 14 \text{ (doubled)} \\ \pm 1.09941 & k = 2, 8, 10, 11, 13, 19 \\ \pm 1.41421 & k = 3, 6, 9, 12, 15, 18 \\ \pm 2.40651 & k = 1, 4, 5, 16, 17, 20 \\ \pm 3.00000 & k = 21 \end{cases}$$

as plotted in Figure 4.

Klein *et al.* found that the HMO secular determinant of all toroidal benzenoids as bucky tubes can be reduced to 2×2 determinants as in the case of the graphite network.^{29,34} The above result reveals that the network of our HBCT belong to this family.³⁵

The topological structure of the cyclic monomer of HBCT is very simple and one can extend this process to the larger members of the series (c) in Figure 1.²⁷ Namely, the next larger member of HBCT can be constructed by joining the 19 benzene-like cyclic structure as in Figure 8. Then by tracing a path as in Figure 7a one can find a Hamiltonian cycle and draw a generalized Heawood graph, $H(114, 15, -15)$, which is composed of 114 vertices with 57-fold rotational symmetry. The eigenvalues can be obtained from Eq. (3) with $n = 57$ and $m=7$.

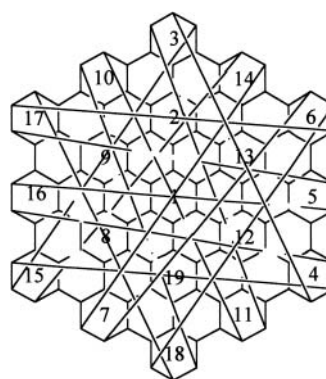


Figure 8. Cyclic structure with 19 benzene rings of the next higher member of HBCT.

TORUS STRUCTURE

It is not difficult to imagine from Figure 7b that this network can be mapped on the surface of a donut without crossing any two bonds. Another way of mapping the HBCT network on a donut surface can be illustrated by the use of Figure 9. Glue the top and bottom edges of the rectangle to make a tube, join its open ends with each

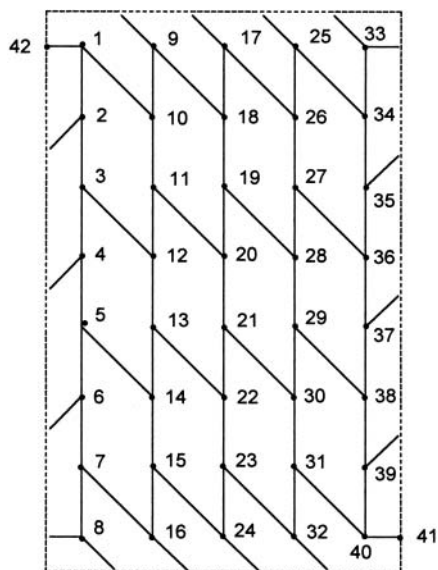


Figure 9. Illustrative drawing of HBCT for showing its mapping on a donut surface. The numbering is the same as in Figure 7.

other by twisting the tube into a ring shape, and then a ring donut comes out.

As has been noted before all the cyclic monomers of HBCT are connected with each other through bridges of a unit length in a topological sense. This means that if each of these seven hexagons is compressed to a node, the skeletal structure of HBCT becomes the complete graph, K_7 . Since HBCT has been shown to be mapped on the surface of a donut, K_7 can thus be embedded in a torus (see Figure 10a).^{17,37} This means that at least seven colors

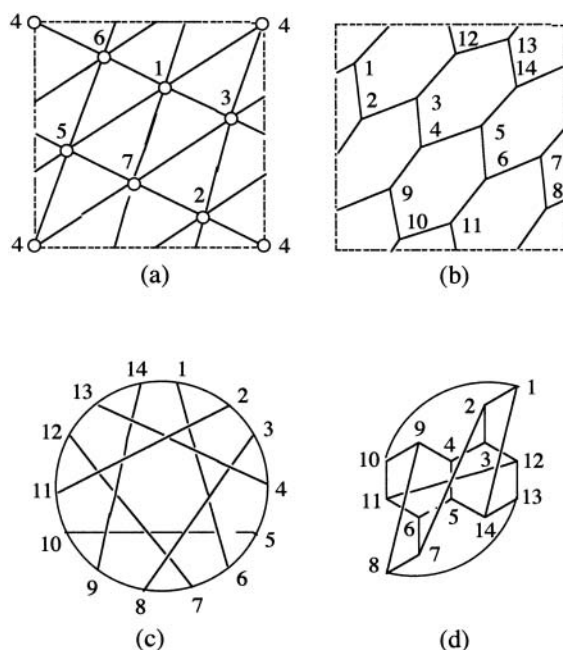


Figure 10. Relation among HBCT, complete graph K_7 (a), its dual (b), the original Heawood graph (c), and the paving unit (d) for the graphite network.

are necessary for painting a given (geometrical) map on a torus, or a donut, so that no two countries of the same color are facing at their border. This is an extension of the famous 4-color problem in a plane or on a sphere.

Further, the dual of K_7 (b) is known to be the unique six-cage,³⁷ or the original Heawood graph (c) denoted by $H(14, 5, -5)$,¹⁸ which can be obtained by tracing the numbers given in (b). Also from (b) one can obtain the paving unit (d) for the graphite network, which however cannot be expressed as MLCFG.¹⁸ This network can be transformed into a monobranched phenarene composed of three pericondensed benzene rings. Although this network can also span the graphite network, its pattern is not unique as in the case of naphthalene and all other polyacenes.

EXTENSION

As suggested from Figure 8 one can extend our analysis along the networks in Figure 1c to graphite,²⁷ and discuss the electronic structure of graphite and also perform model calculations of reactions occurring on its surface. Group-theoretical consideration as Stewart¹⁴ can be extended for these networks.

Study of the perfect matchings of toroidal benzenoids is being underway along the extensive study by Klein and Zhu.^{38–40}

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SAŽETAK

Supersimetrija heksabenzokoronenskoga torusa

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Heksabenzokoronenski torus (HBCT) hipotetska je mreža oblika torusa izvedena pravilnim povezivanjem devet parova perifernih ugljikovih atoma heksabenzokoronenskoga kostura. π -Elektronska struktura te hipotetske konjugirane mreže posjeduje izrazito visoku simetriju (supersimetriju) i slična je grafitnoj mreži. Rabeći metodu temeljenu na teoriji grupa, koju su razvili autori, pokazano je da se 42×42 sekularna determinanta za HBCT može faktorizirati u produkt od 21 kvadratne jednačbe. Autori su naveli brojna zanimljiva matematička svojstva supersimetrije HBCT.