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Leapfrog and Related Operations on Toroidal Fullerenes

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3-valent hexagonal tilings
leapfrog transformation

A 4-valent square tiled toroid is transformed into 3-valent hexagonal (and other polygonal) lattices either by simple cutting procedures or by some more elaborated operations such as leapfrog and related transformations. Tiling or embedding isomers can be interchanged by means of such operations on toroidal maps, for which rigorous definitions and some theorems are given. Parents and products of most important operations are illustrated.

INTRODUCTION

Carbon allotropes, other than ancient graphite and diamond, arose from rational design of highly symmetric molecular structures and appropriate synthesis.[1,2]

In the two last decades, finite molecular cage structures have been synthesized, and characterized from a physico-chemical point of view. They have been functionalized or inserted in some supramolecular compounds.[3-6] Besides the well-known spherical fullerenes, other graphitoids which have excited researchers are carbon nanotubes[7-9] and tori.[10-26]

It is known that a spherical surface cannot be tessellated by a pure hexagonal pattern. In finding structural conditions for preferable fullerenes,[27] the scientists investigated a variety of covering patterns, *e.g.*, combinations of C_5, C_6, C_7, polygons, arranged in different ways, with a view to lowering the total energy of possible molecular structures.[10,26,28] However, the fascination of pure polyhex graphitoids remained. Such structures include cylinders (*e.g.*, open nanotubes), tori and the Klein bottles,[29] the first – and structures that quite possibly are tori – being identified among the products of laser irradiation of graphite.[7,8,30-33]

A toroidal surface can be covered with hexagons by cutting out a parallellogram[13,14,20,23,24] from a graphite sheet, rolling it up to form a tube and finally gluing its two ends to form a torus.

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A method for visualizing a structure for which an adjacency matrix or connection table is already available, is the use of adjacency matrix eigenvectors to find appropriate 3D coordinates of a graph (in particular, here, of a torus).[34–37] The method was previously used in generating spheroidal fullerenes.[38] Polyhex tori are more agreeable to organic chemists (perhaps they offer the pure carbon benzenoid model)[26,39] while the other tessellated tori (*i.e.*, various sized polygons) are expected to appear in supramolecular inorganic compounds (see polyoxometalates).[40]

Diudea[41-45] has recently proposed a procedure for generating polyhex tori starting from a square net embedded on the toroidal surface. In short, a circulant c-folded cycle, lying in a plane perpendicular to the tube, of radius r, runs around the torus, of radius $R > r$. The subsequent n copies of the cycle, equally spaced and joined with edges, point by point, form a square net covering the torus. In all, $c \times n$ points are generated and evenly distributed on the toroidal surface.

The control parameters are c, n, R and r (the last two not being directly involved in the topological characterization of the lattice). The name of the resulting square torus $C_4[c,n]$ includes the polygon size and the c and n dimensions of the lattice. The square torus is next submitted to some cutting procedures (detailed elsewhere)[43,44] providing, after optimization by a molecular mechanics procedure, hexagonal nets or other polygonal tilings, of chemical importance.

In the present paper the attention is focused on operations allowing the transformation of both 4-valent and 3-valent lattices into 3-valent nets that are plausible from a chemical point of view.

SIMPLE OPERATIONS ON A MAP

A map, M is a combinatorial representation of a closed surface.[46,47] Several transformations (*i.e.*, operations) on maps are known and used for various purposes.

Let us denote in a map: v – number of vertices, e – number of edges, f – number of faces and d – vertex degree. An asterisk * will mark the corresponding parameters in the transformed map.

Recall the basic relations in a map:

$$\sum d\, v_d = 2e \tag{1}$$

$$\sum n\, f_n = 2e \tag{2}$$

where v_d and f_n are the number of vertices of degree d and number of n-gonal faces, respectively. The two relations are joined in the famous Euler's formula:

$$v - e + f = 2 - 2g \tag{3}$$

with g being the genus[48] of a graph (*e.g.*, $g = 0$ for a planar graph and 1 for a toroidal graph).

This formula is useful for checking the consistency of an assumed structure.

STELLATION, St, of a face is achieved by adding a new vertex in its center followed by connecting it with each boundary vertex. It is also called a capping operation or triangulation.[49] When all the faces of a map are thus operated, it is referred to as an omnicapping operation. The resulting map shows the relations:

$$\text{St(M):} \quad \begin{aligned} v^* &= v + f \\ e^* &= 3e \\ f^* &= 2e \end{aligned} \tag{4}$$

so that the Euler's relation holds.

DUALIZATION, Du, of a map is built as follows: locate a point in the center of each face. Join two such points if their corresponding faces share a common edge. The new edge is called the edge dual, Du(e) and the transformed map, the (Poincaré) dual Du(M). The vertices of Du(M) represent the faces of M and *vice-versa*.[47] Thus the following relations exist:

$$\text{Du(M):} \quad \begin{aligned} v^* &= f \\ e^* &= e \\ f^* &= v\,. \end{aligned} \tag{5}$$

Dual of the dual recovers the original map: Du(Du(M)) = M.

COMPOSITE OPERATIONS

LEAPFROG, Le, is a composite operation [47,50-52] that can be written as:

$$\text{Le(M)} = \text{Du(St(M))}\,. \tag{6}$$

Within the leapfrog process, the dualization is made on the stellated map. A sequence stellation-dualization rotates parent n-gonal faces by π/n.[51] Figure 1 illustrates Le in case of a square face.

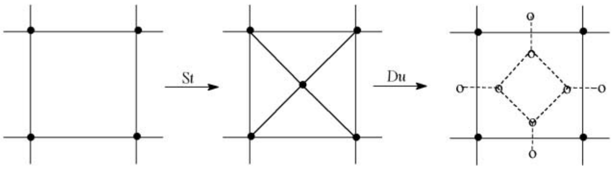

Figure 1. Leapfrog Le operation on a square face; circles denote the vertices in Le transform.

If the map is a d regular graph, the following theorem is true:

THEOREM 1. *The number of vertices in the leapfrog transform Le(M) of M is* d *times larger than in the original map M, irrespective of the type of tessellation.*

The demonstration follows from the observation[42] that each edge in M shares two vertices in Le(M). Thus, keeping in mind Eq. (1), it follows that:

$$v^* = 2e = dv \tag{7}$$

$$v^* / v = dv / v = d\,. \tag{8}$$

Eq. (8) clearly shows no dependency on the type of tessellation. Note that the vertex degree in Le(M) is always 3, as a consequence of the involved stellation. In other words, the dual of a triangulation is a cubic net.[47]

For completion,

$$\begin{aligned} \mathrm{Le(M)}: \quad & v^* = dv = 2e \\ & e^* = 3e \\ & f^* = f + v\,. \end{aligned} \tag{9}$$

A simple example of using Le operation is: Le(Dodecahedron) = Fullerene C_{60}. Leapfrogging can be achieved by a different sequence of simple operations: Le = Tr(Du(M)) where Tr denotes the truncation operation[47] (not discussed in detail herein). An example of the above sequence of operations is: Tr(Icosahedron) = Fullerene C_{60}, where Icosahedron = Du(Dodecahedron). The leapfrog operation can be used to get isolate pentagons in spherical fullerenes.[1,27]

In square tori (Figure 2(a)), the leapfrogging can be used to switch from a 4-valent net to a 3-valent one. The $\pi/4$ rotation, appearing by Le, would produce a rhomboidal RC_4C_8 lattice (Figure 2(c)). The multiplication ratio 4 is conceivable evenly distributed on the two dimensions c and n. When applied to a rhomboidal RC_4 net (Figure 2(b)) the resulting leapfrog transform is a normal HC_4C_8 lattice (Figure 2(d)). In the above symbol, H before the net type C_4C_8 denotes the »horizontal« orientation of the cut edges.

MEDIAL, Me, is an important operation of a map.[42,46,47] It is achieved as follows: put the new vertices as the midpoints of the original edges. Join two vertices if and only if the original edges span an angle. More exactly, the two edges must be incident and consecutive within a rotation path around their common vertex in the original map.

The medial graph is a subgraph of the line-graph.[48] In the line-graph each original vertex gives rise to a complete graph while in the medial graph only a cycle C_d (*i.e.*, a d-membered cycle, d being the vertex degree) is formed. The medial of a map is a 4-valent graph and Me(M) = Me(Du(M)). The transformed parameters are:

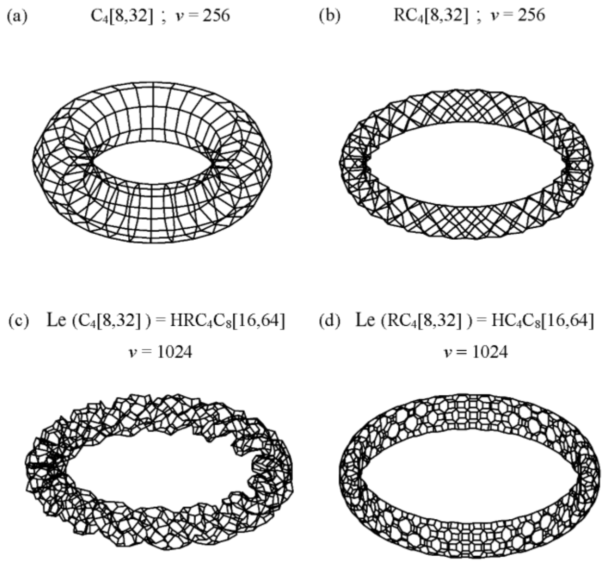

Figure 2. Leapfrog transforms of two 4-valent tori: $C_4[8,32]$ and $RC_4[8,32]$.

$$\begin{aligned} \mathrm{Me(M)}: \quad & v^* = e \\ & e^* = 2e \\ & f^* = f + v\,. \end{aligned} \tag{10}$$

The medial operation rotates parent n-gonal faces by π/n.

DUAL OF THE STELLATION OF A MEDIAL, Dsm. Dual of the stellation of a medial is a new composite operation[42] that can be written as:

$$\mathrm{Dsm\ (M) = Du(St(Me(M)))}\,. \tag{11}$$

Figure 3 illustrates the steps involved by this operation, in the particular case of a square face.

THEOREM 2. *The vertex multiplication ratio in a Dsm transformation is* 2d, *irrespective of the tiling type. It preserves the initial mutual orientation of all parent faces.*

With the observation that each vertex v of M gives rise to twice d new vertices in Dsm(M) it is easily seen that:

$$v^* / v = 2dv / v = 2d \tag{12}$$

and it does not depend on the kind of polygonal faces. The multiplication is twice that induced by Le. Since it consists of simple operations that rotate the parent n-gonal faces by an even number of π/n, the global result of Dsm is the preservation of their original mutual orientation. The transformed parameters are:[42]

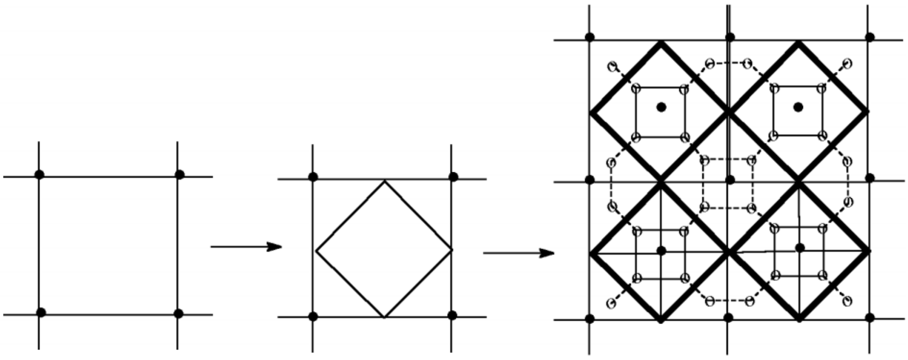

Figure 3. Dual of the stellation of a medial Dsm transformation of a square net.

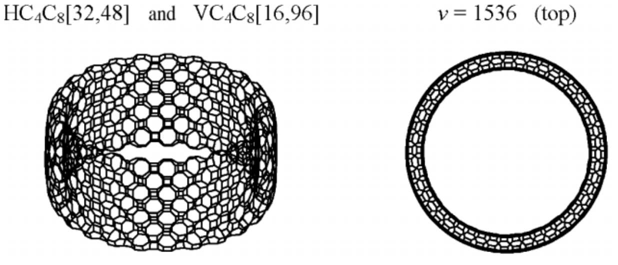

Figure 4. Two possible Dsm transforms of $HC_4[8,24]$: $HC_4C_8[32,48]$ and $VC_4C_8[16,96]$, two different embeddings of the same topological object on 1536 points.

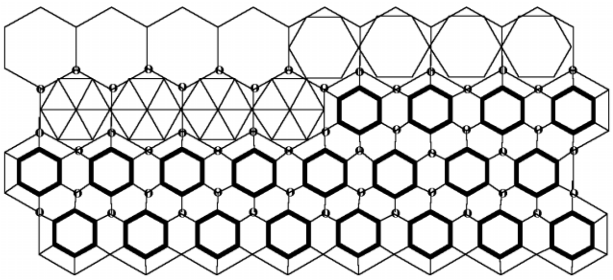

Figure 5. Stages in a quadrupling Q transformation of a polyhex net.

$$\mathrm{Dsm(M)}: \quad v^{*} = 2dv = 4e$$

$$e^{*} = 6e \tag{13}$$

$$f^{*} = f + v + e\,.$$

This operation is particularly applicable to square tori, with a multiplication ratio 8. The expansion is eventually non-isotropic, over the two dimensions ($c \times n = 4 \times 2$, and *vice-versa*, for an H- and a V-net, respectively) as illustrated in Figure 4 for the Dsm transforms of C_4 [8,24].

Note that in square tori the bounding face is an octagon, as expected for a 4-valent regular graph. The pattern is thus a C_4C_8 net (see Figure 3).

The two objects in Figure 4 represent two different embeddings of the same topological object on 1536 points (*i.e.*, atoms): both have 16 × 48 hexes and the same vertex distance degree sequence DDS,[53] given as (vertes contribution to) the Hosoya polynomial[54,55] (see Appendix). Wiener index W (*i.e.*, the sum of all distances in the graph) is, consequently, equal for the both embedding isomers: $W = 33{,}546{,}240$. Also identical are the spectra of eigenvalues of their adjacency matrix.

General formulas for the Hosoya polynomial and Wiener index in tori HC_4C_8 [c,n] and VC_4C_8 [c,n] are given elsewhere.[56]

Q-TRANSFORMATION. There exists another transformation that preserves the initial orientations of all parent faces in the map. It is called the quadrupling transformation Q.[51,57] The Q operation can be viewed as a particular case of Dsm:

$$\mathrm{Q(M)} = \mathrm{Du(St(Mer(M)))} \tag{14}$$

with Mer being a reduced medial, where the face resulted (by Me operation) around each original vertex collapses into this vertex, so preserving its original valency. It is illustrated for a hexagonal net in Figure 5.

THEOREM 3. *The vertex multiplication ratio in a Q transformation is* d + *1 irrespective of the tiling type of the original map.*

With the observation that for each vertex v in M results d new vertices in Q(M) and the old vertices are preserved, the demonstration is immediate:[42]

$$v^{*} = vd + v \tag{15}$$

and the multiplication ratio:

$$v^{*} / v = v(d+1) / v = d + 1\,. \tag{16}$$

Q operation involves two π/n rotations, so that the initial orientation of the polygonal faces is conserved.

The transformed parameters are:[42]

$$Q(M): \quad v^{*} = v + 2e = v + dv$$

$$e^{*} = 4e \tag{17}$$

$$f^{*} = f + e\,.$$

This operation works well in trivalent maps (*e.g.*, in polyhex tori – see below), with 3 + 1 = 4, the multiplication ratio, and conserving the regular degree 3. Conversely, in a square net, this operation leads to nonregular graphs (degree 3 and 4) and therefore it is useless.

LEAPFROGGING POLYHEX TORI

When the leapfrog operation is applied to polyhex tori, two cases appear, function of the starting lattice: HC_6 and VC_6. The dualization step will decide the type of the leapfrog product.

(i) CASE OF HC_6 PATTERN. The leapfrog product is an acenic (*i.e.*, armchair) net, herein called a VC_6 pattern. The process acts in the sense of expanding, three times, the *n*-dimension (thus producing a minimal modification of the net) of a torus. Figure 6 illustrates the stages occurring in the leapfrog transformation of an HC_6 net. It appears more clear after geometry optimization (Figure 7).

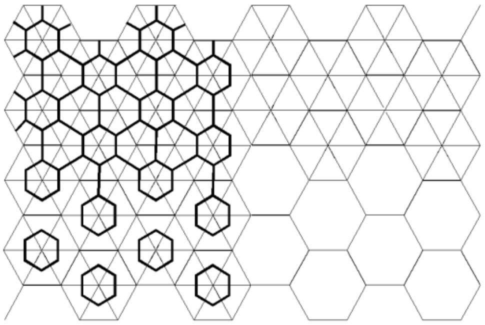

Figure 6. Stages in the leapfrog transformation of a HC_6-pattern.

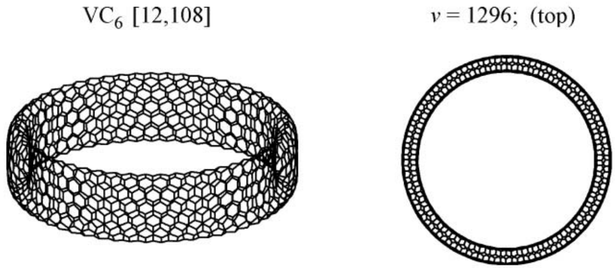

Figure 7. Leapfrog transform of $HC_6[12,36]$: $VC_6[12,108]$.

(ii) CASE OF VC_6 PATTERN. The leapfrog product is now a phenacenic, HC_6 patterned net (see Figures 8 and 9). In this case, the leapfrog transformation expands (three times) the *c*-dimension of a torus.

Observe that, at a limited value of *n*, the increasing *c*-dimension provides tubes with a flattened shape (Figure 9). It is the case of the so-called »elongated« tori.[12]

Q operations are useful in polyhex tori for preserving the pattern: HC_6 or VC_6. Figure 10 illustrates such a transformation. The two objects in this figure are embedding isomers, with different topology, as shown by their (vertex) Hosoya polynomials and Wiener numbers (see Appendix). A more simple example of using the Q operation is: Q(Dodecahedron) = [80]Fullerene.

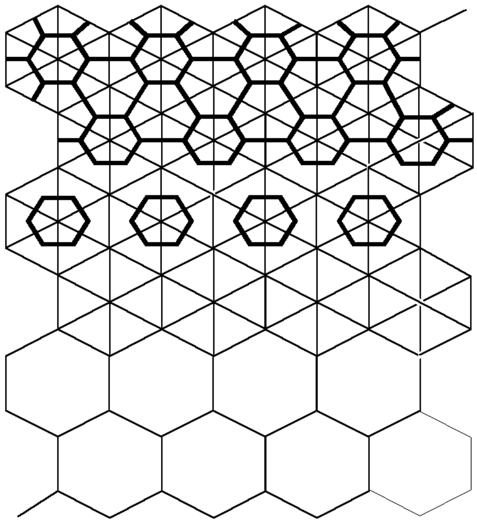

Figure 8. Stages in the leapfrog transformation of a VC_6-pattern.

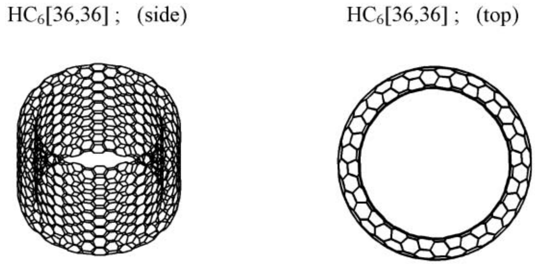

Figure 9. Leapfrog transform of $VC_6[12,36]$: $HC_6[36,36]$.

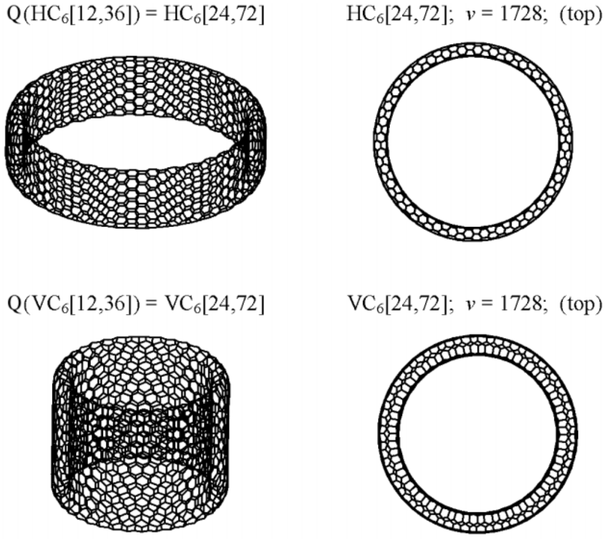

Figure 10. Quadrupling transforms of $HC_6[12,36]$ and $VC_6[12,36]$

In contrast to the C_4C_8 series, the C_6 tori clearly show different topology for embedding isomers, even in case they have the same number of hexes on each dimension. As an example, the pair (HC_6 [24,72]; VC_6 [12,144]) is given: the two objects differ both in Hosoya polynomial and Wiener index (see Appendix).

CONCLUSIONS

Square tori can be used for generating hexagonal (and combined polygonal) tori, either by appropriate cutting procedures or by leapfrog and related operations.

Leapfrog acting on a non-isotropic polyhex lattice leads to the mutual interchanging of its twin patterns: HC_6 and VC_6, respectively. Q operation, applied in polyhex tori, preserves the original pattern orientation. The operations presented above can also be described by »unit-cell« operations, as will be shown in a future paper.

The involvement of such operations in the energetic of toroidal objects has been already discussed in the literature.[14,23,25,46,52,58]

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APPENDIX
HOSOYA POLINOMIALS AND WIENER INDEX IN SOME TORI

HC_4C_8 [32,48] and VC_4C_8 [16,96] (16 × 48 hexes):

$$H(i,x) = 1 + 3x + 5x^2 + 8x^3 + 11x^4 + 13x^5 + 16x^6 + 19x^7 + 21x^8 + 24x^9 + 27x^{10} + 29x^{11} + 32x^{12} + 35x^{13} + 37x^{14} + 40x^{15} + 42x^{16} + 41x^{17} + 40x^{18} + 39x^{19} + 37x^{20} + 36x^{21} + 35x^{22} + 33x^{23} + 32x^{24-47} + 31x^{48} + 28x^{49} + 24x^{50} + 20x^{51} + 16x^{52} + 12x^{53} + 8x^{54} + 4x^{55} + x^{56}$$

$W = 33,546,240.$

HC_6 [24,72] (12 × 72 hexes):

$$H(i,x) = 1 + 3x + 6x^2 + 9x^3 + 12x^4 + 15x^5 + 18x^6 + 21x^7 + 24x^8 + 27x^9 + 30x^{10} + 33x^{11} + 35x^{12} + 35x^{13} + 34x^{14} + 33x^{15} + 32x^{16} + 31x^{17} + 30x^{18} + 29x^{19} + 28x^{20} + 27x^{21} + 26x^{22} + 25x^{23} + 24x^{24-71} + 12x^{72}$$

$W(HC_6\ [24,72]) = 5.4736128 \times 10^7$

VC_6 [24,72] (24 × 36 hexes):

$$H(i,x) = 1 + 3x + 6x^2 + 9x^3 + 12x^4 + 15x^5 + 18x^6 + 21x^7 + 24x^8 + 27x^9 + 30x^{10} + 33x^{11} + 36x^{12} + 39x^{13} + 42x^{14} + 45x^{15} + 48x^{16} + 51x^{17} + 54x^{18} + 57x^{19} + 60x^{20} + 63x^{21} + 66x^{22} + 69x^{23} + 59x^{24} + 48x^{25-35} + 47x^{36} + 44x^{37} + 40x^{38} + 36x^{39} + 32x^{40} + 28x^{41} + 24x^{42} + 20x^{43} + 16x^{44} + 12x^{45} + 8x^{46} + 4x^{47} + x^{48}$$

$W(VC_6\ [24,72]) = 3.6820224 \times 10^7$

VC_6 [12,144] (12 × 72 hexes):

$$H(i,x) = 1 + 3x + 6x^2 + 9x^3 + 12x^4 + 15x^5 + 18x^6 + 21x^7 + 24x^8 + 27x^9 + 30x^{10} + 33x^{11} + 29x^{12} + 24x^{13-71} + 23x^{72} + 20x^{73} + 16x^{74} + 12x^{75} + 8x^{76} + 4x^{77} + x^{78}$$

$W(VC_6\ [12,144]) = 5.8347648 \times 10^7$

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SAŽETAK

»Leapfrog« i srodne operacije na toroidalnim fullerenima

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Četverovalentni, kvadratima parketirani toroid dade se transformirati u trovalentnu heksagonalnu rešetku i druge poligonalne rešetke uporabom jednostavnoga rezanja ili složenijih »leapfrog« i srodnih operacija. Primjenom ovih operacija jedni se parketirani izomeri prevode u druge, a za te operacije dane su stroge definicije i nekoliko teorema. Za najvažnije operacije prikazana su početna i konačna parketiranja.