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## Toroidal Fullerenes from Square Tiled Tori

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## Toroidal Fullerenes from Square Tiled Tori<sup>#</sup>

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### Abstract

**Motivation.** Novel carbon allotropes, with finite molecular structure, including spherical (classical) fullerenes, capsulenes, tubulenes, barrellenes, and torrenes are nowadays currently produced and investigated. These classes of compounds have beautiful architectures and show unusual properties that are very promising for the development of nanotechnologies.

**Method.** A novel method for computer generation of toroidal fullerenes, based on appropriate cuttings performed on square tori, is herein presented. The obtained structures were investigated with molecular mechanics and semiempirical PM3 approaches.

**Results.** Our method provides toroidal objects representing pertinent models for real molecular structures.

**Conclusions.** A novel way in constructing toroidal fullerenes (namely by operating on a square–like net, embedded onto a toroidal surface) is added to the well–known graphite zone–folding and adjacency matrix eigenvector procedures. Preliminary data show torranes (fully hydrogenated) rather than torrenes (aromatic or olefinic) as stable chemical toroidal structures.

**Availability** The software program TORUS 1.0 (in DELPHI 4.0) is available on request.

**Keywords.** Fullerenes; tori; leapfrog; molecular mechanics; PM3.

### Abbreviations and notations

$d_{ext}$ , external diameter of the torus

$d_{int}$ , internal diameter of the torus

$h$ , height of the torus

HL–GAP, the HOMO–LUMO gap

IPR, isolated pentagon rule

MM+, a molecular mechanics program from HyperChem

rms, root mean square value

$w$ , wall thickness of the torus

## 1 INTRODUCTION

Buckminsterfullerene, C<sub>60</sub>, represents the prototype of a vast class of new carbon cage molecules collectively termed as fullerenes, stimulating the imagination and efforts of scientists in achieving beautiful architectures on the nanometer scale [1–3]. Fullerene chemistry is nowadays a highly

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active research field [4–6]. Carbon allotropes with finite molecular cage structures have been functionalized or inserted into supramolecular assemblies [7–9].

It is worth to recall some historical steps [1] in the hard and finally fruitful way from theory to synthesis of the most rational class of chemical compounds: fullerenes. Early in 1966, David Jones [10] published in *New Scientist* “The Inventions of Daedalus” where he made the prescient suggestion that the high temperature graphite production might be modified to generate graphite balloons. In 1970, Osawa [11] published in *Kagaku* (in Japanese) his conjecture on the possible stability of the C<sub>60</sub> molecule, inspired by the beautiful symmetry of a modern football. In 1972 Bochvar and Gal’pern [12] have presented the first Hückel calculation on C<sub>60</sub>. Another Hückel result was due to Davidson, in 1981 [13]. Attempts to derive an IUPAC name for the hydrogenated species C<sub>60</sub>H<sub>60</sub> were made by Castells and Serratos in 1983 and 1986 [14] and examples can continue.

In 1991 Iijima [17] discovered graphitic nanotubes, a kind of expansion of the C<sub>60</sub> cage in one direction. It was the beginning of a race to the most perfect possible carbon fiber: effectively a single crystal of carbon in one linear dimension. Some other theoretical papers followed [18] and finally, in 1997, fullerene crop circles have been observed in laser-grown single-wall carbon nanotubes by Liu *et al.* [19]. Such toroidal nanotubes offer a prototype of study (a ring of quantum wire with a turning current, thus creating magnetic moment) and a promise for novel unexpected applications.

C<sub>60</sub>, with truncated icosahedron symmetry, is the smallest spherical cage without abutting pentagons. An *isolable fullerene* should avoid strained or antiaromatic rings, such as fused pentagons (*e.g.*, pentalene). This finding led to the IPR (Isolated Pentagon Rule) [18]. In the view of eluding such undesirable structures the leapfrog transformation was proposed. It results in isolating pentagons (reminding the pentagons of dodecahedron) by surrounding hexagons.

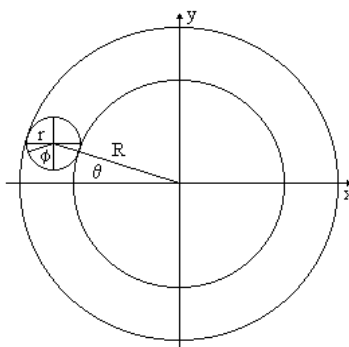
Since a spherical surface cannot be tiled by pure hexagonal pattern [20,21], the scientists considered other surfaces capable to allow a full polyhex tessellation. Such surfaces are cylinders (*e.g.*, open nanotubes) and tori [22–30], both of them identified in the products of laser irradiation of graphite [17,19]. A torus obeys the Euler’s formula:  $v - e + f = 2 - 2g$  ( $v$ ,  $e$ ,  $f$ ,  $g$  being respectively the number of vertices, number of edges, number of faces, and genus) with genus equal to unity while a sphere or a cylinder are of genus zero. This formula is useful for checking the consistency of an assumed structure.

This paper describes a novel way of generating polyhex tori, starting from square-like tori. Leapfrog transformation along with the energetic characterization of some classes of tori are presented.

## 2 CONSTRUCTION OF POLYHEX TORI

Covering a toroidal surface by hexagons is related to the tessellation of an equivalent planar parallelogram [21,26,28,29]. A torus  $T_{p,q,t}$  is obtained from  $p \times q$  hexagons stacked in a  $p \times q$ -parallelogram, whose opposite edges are glued in order to form a tube. Next, the two ends of the tube are glued together, eventually rotated by  $t$  hexagons before gluing, to form the torus. An alternative to the parallelogram procedure is the use of adjacency matrix eigenvectors in finding appropriate triplets, *i.e.*, 3D coordinates of a graph (in particular, a torus) [31]. The method was previously used in generating spheroidal fullerenes [32,33].

Our construction starts from a quadrilateral net embedded on the toroidal surface, generated according to an elementary geometry (see ref. [34]). A torus  $T_{c,n}$  is a lattice obtained by circulating a  $c$ -membered cycle along another cycle: its  $n$  images together with the edges joining (point by point) the subsequent images form a polyhedral torus tiled by some square patterns (Figure 1).



**Figure 1.** Construction of a toroidal surface.

The equations used for generating the toroidal surface are:

$$\begin{aligned}x &= \cos(\theta)(R + r \cos \varphi) \\y &= \sin(\theta)(R + r \cos \varphi) \\z &= r \sin \varphi\end{aligned}\tag{1}$$

The problem is now to change the squares into hexagons or other tiling patterns, suitable from a chemical point of view. In this respect, several cutting procedures were developed. A cutting operation consists of deleting appropriate edges in a square-like net in order to produce some larger polygonal faces. By deleting each second *horizontal* edge and alternating edges and cuts in each second vertex row it results in a standard  $h,C_6$  pattern (Figure 2,a). After optimizing by a molecular mechanics program, angular hexagonal (phenanthrenoid) pattern appears on the torus. By following the same algorithm as above, but operating vertically, a standard  $v,C_6$  pattern (Figure 2,b) is generated. After optimization an isomeric linear (anthracenoid) pattern is obtained.

Note that each hexagon consumes exactly two squares in the square lattice. By construction, the

number of hexagons in the  $h, C_6$  pattern is half the number of squares on dimension  $c$  of the torus  $T_{c,n}$  while in the  $v, C_6$  pattern the reduced number of hexagons appears on dimension  $n$ . We have to consider that the above cutting procedure leaves unchanged the number of vertices in the original square-like torus. The name of a polyhex torus, thus generated, has to remind the type of cutting,  $h$  or  $v$ , as well as the type of cycles occurring in a given pattern.

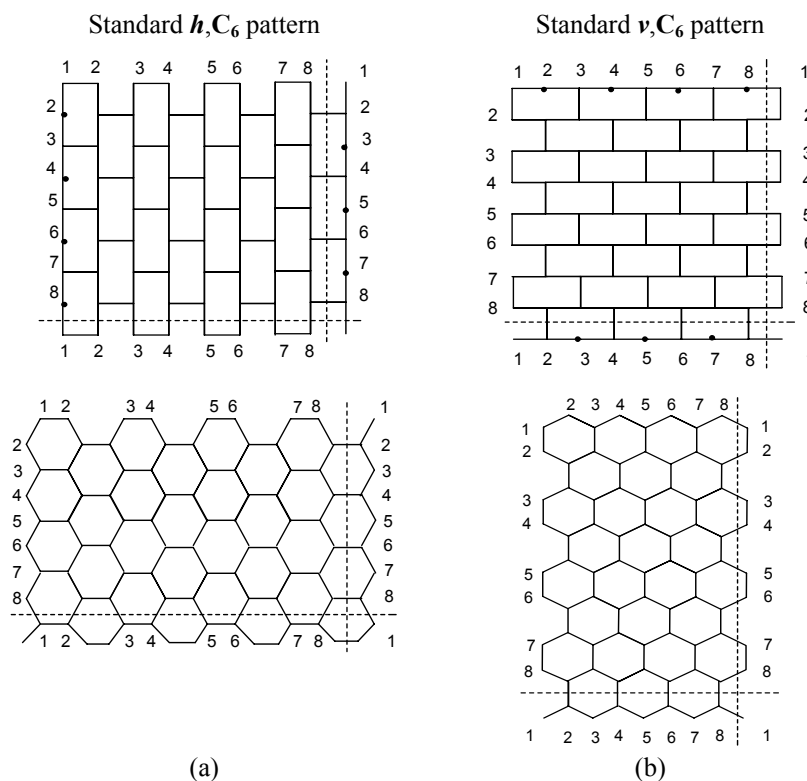


Figure 2. Standard  $C_6$  patterns.

### 3 OTHER PATTERN CONSTRUCTIONS

In tessellating a toroidal surface, some other patterns have been considered. An alternating  $C_4, C_8$  pattern was depicted in ref. [23] (see also ref. [35]). In our procedure, this pattern results by following the principle of alternating edges and cuts and keeping the same any two subsequent rows (see Figure 3). This pattern was used for tiling spherical fullerenes [36]. In order to reduce the strain tension in pure polyhex tori, a number of pentagons and heptagons were introduced [23]. When a pure  $C_5, C_7$  pattern is used, the lattice is called azulenoïd [13]. The pentalene (*i.e.*, two fused five-membered rings) apparition is not a problem in tori, since a more pronounced curvature occurs in such structures (see below), in comparison with the spheroidal fullerenes. In our procedure, the construction of a pure  $C_5, C_7$  pattern needs four rows of square faces, namely a  $(0 \bmod 4)$  lattice as presented in Figure 4. In the case of a  $(2 \bmod 4)$  network it results a  $C_5, C_6, C_7$  pattern (Figure 5). In the above constructions, non-twisted nets are obtained. Excepting the patterns involving  $C_5$  and  $C_7$ ,

our tori are clearly non–twisted. This fact is in contrast to the parallelogram procedure, where even for  $t = 0$  (see above) some twisting (*e.g.* an angle of  $\pi / 6$ ) appears.

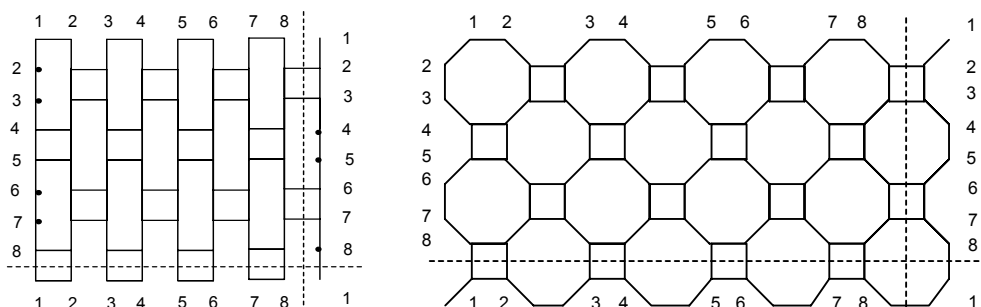


Figure 3. A  $C_4, C_8$  pattern.

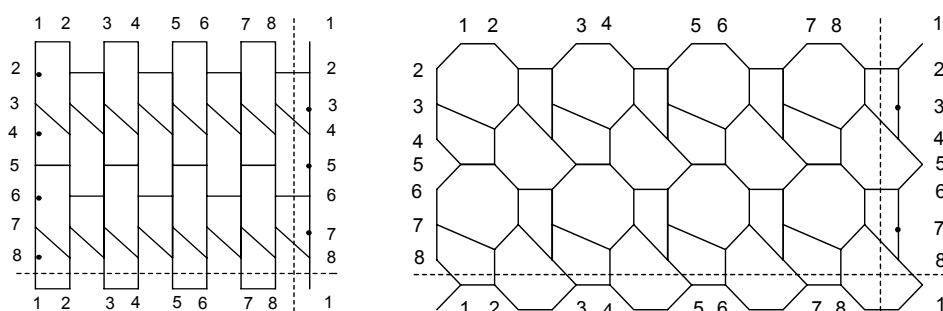


Figure 4. A  $C_5, C_7$  pattern.

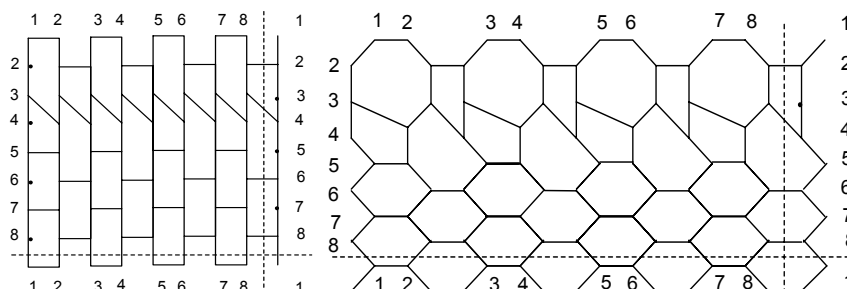
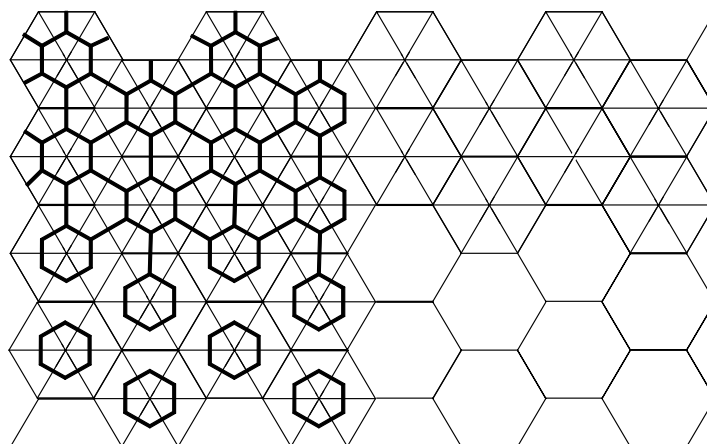


Figure 5. A  $C_5, C_6, C_7$  pattern.

## 4 LEAPFROGGING POLYHEX TORI

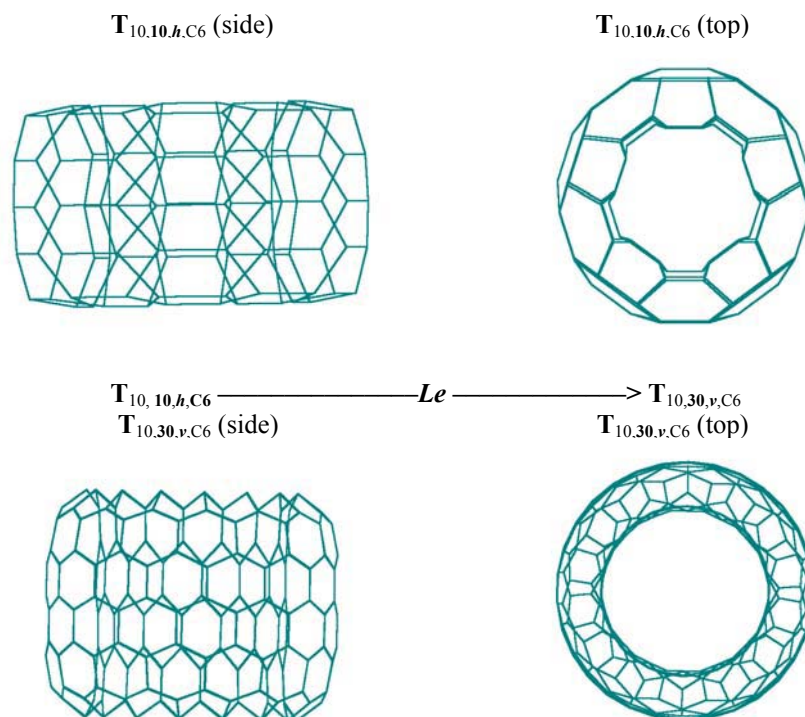
The leapfrog transformation of a map (*i.e.*, a combinatorial representation of a closed surface) involves the omnicapping (triangulation) of its faces followed by dualization [37–39]. Omnicapping a map consists of adding a new vertex in the center of each face and connecting it with each boundary vertex. Dualization is made by locating a point in each face and joining two points if their corresponding faces share an edge. Leapfrogging proceeds with dualization of the stellated (omnicapped) transform of the map. In polyhex tori, two cases appear, depending on the starting lattice:  $h, C_6$  and  $v, C_6$ . The dualization step will decide the type of the leapfrog product. In the case of the  $h, C_6$  pattern (angular isomer), the product is an anthracenoid (linear isomer) net, which in our

approach is equivalent to a  $\nu, C_6$  pattern. The leapfrog operates in the sense of expanding (three times) the  $n$ -dimension of a torus. Figure 6 illustrates the stages occurring in the leapfrog transformation of an  $h, C_6$  net.

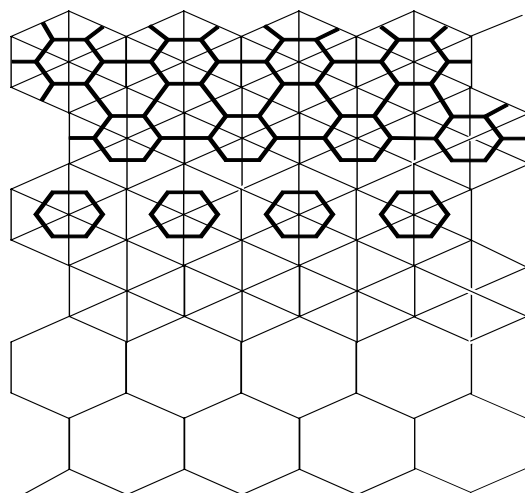


**Figure 6.** Stages in the leapfrog transformation of an  $h, C_6$  pattern.

As illustrated below, it appears more clear after geometry optimization that a pure,  $\nu, C_6$  patterned,  $T_{10,30,\nu,C_6}$  is obtained from the smaller,  $h, C_6$ -patterned,  $T_{10,10,h,C_6}$ .

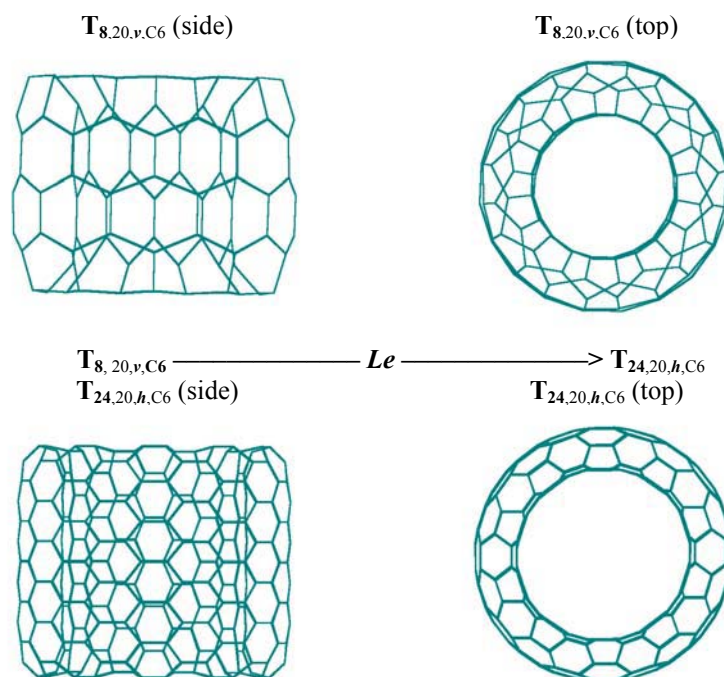


In the case of the  $\nu, C_6$  pattern (linear isomer) the product is now a phenanthrenoid,  $h, C_6$  net (Figure 7). In this case, the leapfrog transformation acts by expanding (three times) the  $c$ -dimension of a torus (see above).



**Figure 7.** Stages in the leapfrog transformation of a  $v,C_6$  pattern.

A nice example is given in the following. Observe that, as the  $c$ -dimension increases, the torus becomes more flattened.



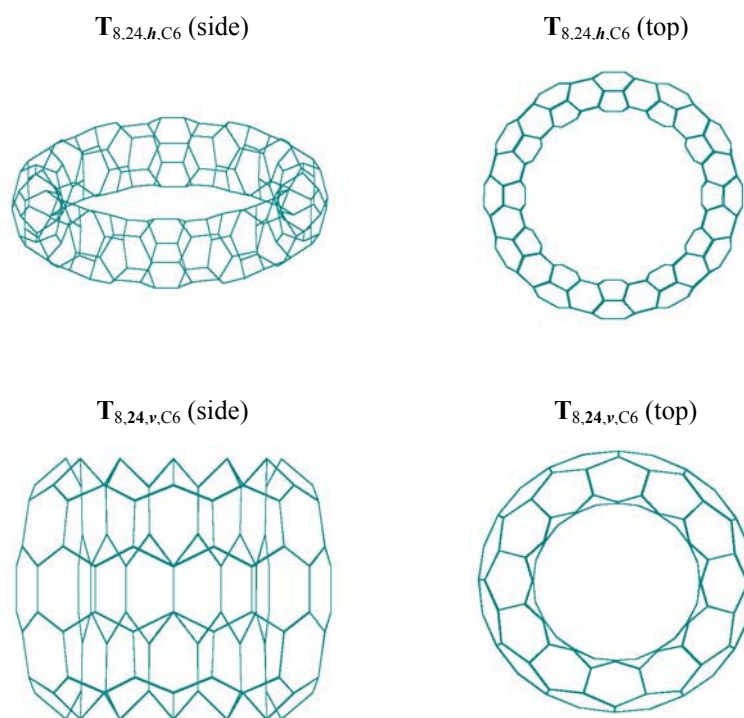
Concluding, the leapfrog transformation of the non-isotropic polyhex lattice leads to the mutual interchanging of its twin patterns  $h,C_6$  and  $v,C_6$ , respectively. Different stability is expected for the different linear and angular isomers, as shown in the next sections.

## 5 MOLECULAR MECHANICS CALCULATIONS

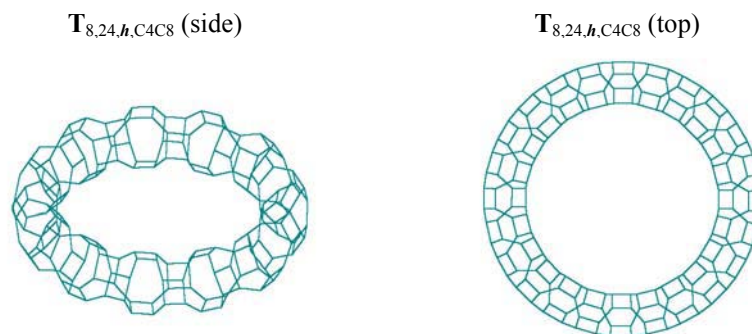
As a consequence of various pattern coverings for a toroidal surface, several isomers (different patterned lattices) are expected for a given  $T_{c,n}$  torus. Our computer program enabled us to generate

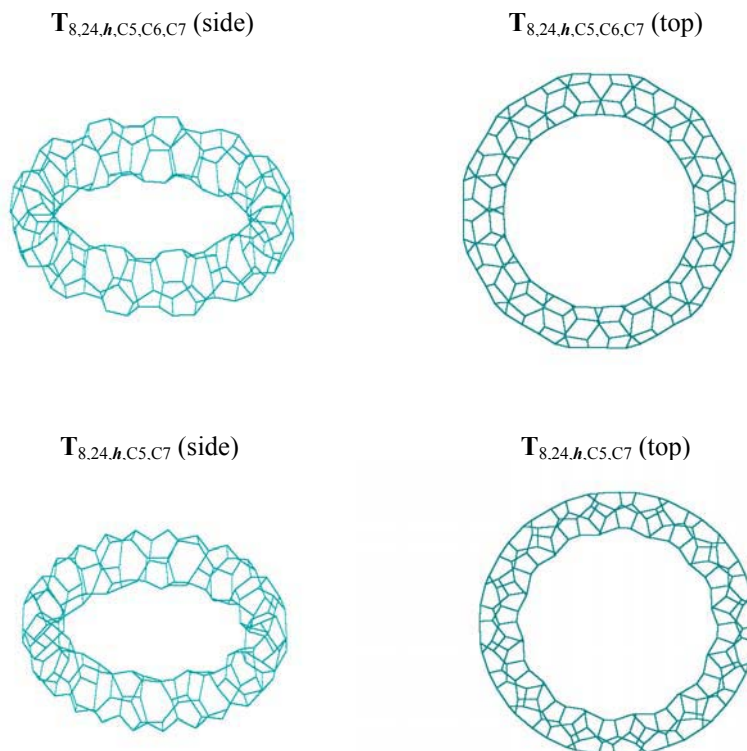


tori with the above described tessellation. The interest is now to find structures plausible from the point of view of chemistry, namely plausible molecules. In a first approximation, we calculated the total energy, as provided by molecular mechanics calculations. The structures considered here (and illustrated below) are isomers of  $T_{8,24}$ , having  $8 \times 24 = 192$  vertices (carbon atoms). They are sufficiently large to minimize the strain energy given by a more pronounced curvature of a toroidal, compared to a spherical surface. Each structure is given as side view and top view.



The value shown by  $T_{8,24,h,C4,C8}$  (entry 6) is a normal one, since small, strained  $C_4$  rings are present. The mixed pattern  $C_5,C_6,C_7$  was considered as an *abnormality* statistically occurring in a polyhex isomer, particularly in large structures. This pattern, as well as the full  $C_5,C_7$  lattice, shows some degree of twisting, in comparison to the standard  $C_6$  patterns. However, in the case of the  $C_5,C_6,C_7$  pattern the strain energy (Table 1, entry 8) is even lower than that of the polyhex isomers (Table 1, entries 2 and 4). Among the discussed structures, the anthracenoid  $T_{8,24,v,C6}$  (entry 4) shows the highest energy (equivalent with highest instability).





Interesting results were obtained when we have considered perhydro–tori, (totally hydrogenated hydrocarbons), called toranes by analogy to alkanes. Such structures, with no  $\pi$  bonds, show low reactivity (*paraffinum*, in Latin) and no aromatic character (see the next section). Toranes from entries 1, 7 and 9 of Table 1 exhibit a lower energy (a higher stability), in comparison with the corresponding pure carbon tori. In the case of  $\mathbf{T}_{8,24,v,C6}$  and  $\mathbf{T}_{8,24,h,C4C8}$  (entries 3 and 5) the hydrogenation results in an exacerbating instability, suggesting a more eclipsed disposition of the hydrogen atoms. An evaluation of lattice dimensions is possible from the optimized geometries. The computed values presented in Table 1 are: internal diameter  $d_{int}$ , external diameter  $d_{ext}$ , wall thickness  $w$ , and height  $h$  (in Ångstroms). In the case of hydrogenated structures, the lattice dimensions refer to the skeleton only, the hydrogen atoms being disregarded. Even so, the lattice appear as somewhat expanded, and no exception was observed.

At the end of this section we present in Figure 11 two polyhex tori, showing complementary dimensions, as a possible assembly (host–guest) of isomers into a nanodevice. Their dimensions are:

$$\mathbf{T}_{20,30,C6} (d_{int} = 18.18; d_{ext} = 23.56; w = 2.69; h = 10.73)$$

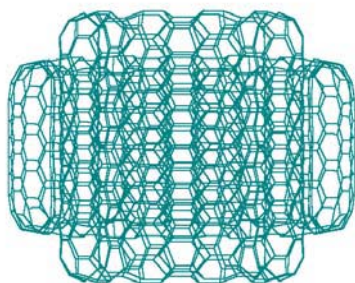
$$\mathbf{T}_{30,20,C6} (d_{int} = 11.42; d_{ext} = 16.61; w = 2.65; h = 16.90)$$

Some enlarged  $d_{int} = 19.66$  of  $\mathbf{T}_{20,30,C6}$  is plausible to accept the guest ( $\mathbf{T}_{30,20,C6}$  of  $d_{ext} = 16.61$ ) into its central hole to form a double layer (of 1200 atoms) assembly.

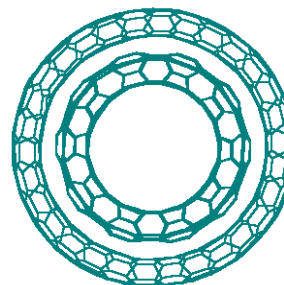
**Table 1.** Data for  $T_{8,24}$ ; Energy E (MM+; kcal/mol; rms = 0.1 ), Internal Diameter  $d_{int}$ , External Diameter  $d_{ext}$ , Wall Thickness  $w$  and Height  $h$  (in Ångstroms)

No	Torus	E (MM+)	$d_{int}$	$d_{ext}$	$w$	$h$
1	8,24, <b>h</b> ,C <sub>6</sub> ,H	2766.56	14.70	20.91	3.11	3.93
2	8,24, <b>h</b> ,C <sub>6</sub>	3544.04	12.94	18.67	2.87	3.54
3	8,24, <b>v</b> ,C <sub>6</sub> ,H	5867.49	7.65	13.34	3.09	8.11
4	8,24, <b>v</b> ,C <sub>6</sub>	5382.92	7.25	11.50	2.37	7.63
5	8,24, <b>h</b> ,C <sub>4</sub> ,C <sub>8</sub> ,H	4395.36	15.58	22.11	3.53	3.83
6	8,24, <b>h</b> ,C <sub>4</sub> ,C <sub>8</sub>	3777.41	14.02	19.62	2.98	3.27
7	8,24, <b>h</b> ,C <sub>5</sub> ,C <sub>6</sub> ,C <sub>7</sub> ,H	2255.72	15.05	21.37	3.41	3.27
8	8,24, <b>h</b> ,C <sub>5</sub> ,C <sub>6</sub> ,C <sub>7</sub>	3081.12	13.61	19.26	3.06	3.40
9	8,24, <b>h</b> ,C <sub>5</sub> ,C <sub>7</sub> ,H	3669.68	15.09	21.67	3.29	3.52
10	8,24, <b>h</b> ,C <sub>5</sub> ,C <sub>7</sub>	4529.19	13.82	19.82	2.67	3.13

$T_{20,30,C6}$  &  $T_{30,20,C6}$  (side)



$T_{20,30,C6}$  &  $T_{30,20,C6}$  (top)



**Figure 11.** A double layer assembly of 1200 atoms.

## 6 SEMIEMPIRICAL COMPUTATIONS

A preferable fullerene [18] obeys the isolated pentagon rule [40,41]. It means that, for higher stability, a trivalent net, embedded on the sphere, should avoid strained or antiaromatic rings, such as triangles, squares or abutting pentagons (*i.e.*, pentalene, the boundary of which is an 8-membered, antiaromatic cycle). Four membered rings on the surface of fullerenes are, however, not completely excluded as recent molecular orbital calculations have shown [36,42]. Actually, heterofullerenes containing only four and six membered rings could be even more stable than their carbon analogues [43–45]. In order to assess the effect of other than six membered rings on the toroidal surface as well as that of the saturation, we have performed semiempirical molecular orbital calculations at the PM3 level on a set of  $T_{8,24}$  systems. Table 2 summarizes the results of single point calculations (at the geometry obtained at the MM+ level) on various members of this series along with those obtained after full optimization at the PM3 level.

We have to mention that toranes are far more stable than the corresponding pure carbon structures (see Tables 1 and 2); this fact is in line with the results of *ab initio* and semiempirical calculations carried out on the fullerene–fullerane systems [45,46]. The HOMO–LUMO gaps (both for the single point calculated as well as the optimized species) increase on going from torenes to

toranes, suggesting a kinetic stabilization. This finding can be interpreted in terms of localization of the surface electron pairs of toranes in the C–H bonds of toranes with the subsequent decrease of the surface interelectronic repulsions.

The results obtained by us suggest that the C<sub>5</sub>,C<sub>6</sub>,C<sub>7</sub> systems (Table 2, entries 5, 6 and 12, 13) should be thermodynamically more stable than other isomers of T<sub>8,24</sub> containing pure (C<sub>4</sub>,C<sub>8</sub>), (C<sub>6</sub>) or (C<sub>5</sub>,C<sub>7</sub>) lattices. This result is in agreement with those obtained by other authors [28,31], showing that insertion of equal number of pentagonal and heptagonal defects might reduce the strain energy.

**Table 2.** PM3 Calculation for T<sub>8,24</sub> of Various Patterns: Enthalpy of Formation ΔH<sub>f</sub> (kcal/mol), HOMO, LUMO and HOMO–LUMO Gap HL–GAP (eV)

	Torus T <sub>8,24</sub>	ΔH <sub>f</sub>	HOMO	LUMO	HL–GAP
1	<i>h</i> ,C <sub>6</sub> ,H	2554.00	–9.108	1.105	10.213
2	<i>h</i> ,C <sub>6</sub> ,H <sup>a</sup>	2403.50	–9.010	0.650	9.660
3	C <sub>4</sub> ,C <sub>8</sub> ,H	2518.09	–9.707	1.126	10.833
4	C <sub>4</sub> ,C <sub>8</sub> ,H <sup>a</sup>	2289.55	–9.500	1.240	10.740
5	C <sub>5</sub> ,C <sub>6</sub> ,C <sub>7</sub> ,H	1974.57	–9.170	1.898	11.068
6	C <sub>5</sub> ,C <sub>6</sub> ,C <sub>7</sub> ,H <sup>a</sup>	1811.93	–9.120	1.960	11.080
7	C <sub>5</sub> ,C <sub>7</sub> ,H	4264.05	–9.175	0.766	9.940
8	<i>h</i> ,C <sub>6</sub>	7114.86	–7.848	–4.235	3.613
9	<i>h</i> ,C <sub>6</sub> <sup>a</sup>	6301.44	–8.062	–3.790	4.272
10	C <sub>4</sub> ,C <sub>8</sub>	8913.97	–8.308	–4.629	3.679
11	C <sub>4</sub> ,C <sub>8</sub> <sup>a</sup>	7036.41	–9.031	–2.492	6.539
12	C <sub>5</sub> ,C <sub>6</sub> ,C <sub>7</sub>	6906.63	–9.126	–4.276	4.850
13	C <sub>5</sub> ,C <sub>6</sub> ,C <sub>7</sub> <sup>a</sup>	5790.62	–9.122	–2.951	6.171
14	C <sub>5</sub> ,C <sub>7</sub>	11293.72	–9.035	–3.998	5.037

<sup>a</sup> Values corresponding to the optimized structures at the PM3 level

The semiempirical PM3 [47] calculations have been carried out with SPARTAN 5.0 [48] on an Octane Silicon Graphics machine, and GAMESS–US [49] installed under LINUX on a Pentium III system. Molecular mechanics (MM+ force field) optimizations have been performed with HyperChem 4.5 from HyperCube [50].

## 7 CONCLUSIONS

Toroidal fullerenes, along with tubulenes and classical spherical fullerenes, are the subject of intensive interdisciplinary research in physics, chemistry, and nanotechnology. In this paper a third way in constructing tori, namely by transforming a square–like net (embedded onto a toroidal surface) into polyhex and/or variously tiled lattices, is added to the well–known graphite zone–folding and adjacency matrix eigenvector procedures. The structures thus generated become plausible candidates to the real molecule status as soon as they are optimized with a molecular mechanics or, better, with a quantum chemical computer program. Preliminary data enabled us to propose toranes (fully hydrogenated) rather than torenes (aromatic or olefinic) as possible chemical tessellating of a toroidal surface. Further research is directed towards finding the equivalence of our

structures to the canonical representation [21] and construction of aggregate supramolecular assemblies.

## Acknowledgment

The authors acknowledge the financial support of this research by the Romanian CNCSIS 2001.

## Supplementary Material

The structures given in Tables 1 and 2 are collected in the archive Diudea.zip.

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