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Omega Polynomial in Polybenzene Multi Tori

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Abstract. The polybenzene units BTX_48, X=A (armchair) and X=Z (zig-zag) dimerize forming "eclipsed" isomers, the oligomers of which form structures of five-fold symmetry, called multi-tori. Multi-tori can be designed by appropriate map operations. The genus of multi-tori was calculated from the number of tetrapodal units they consist. A description, in terms of Omega polynomial, of the two linearly periodic BTX-networks was also presented.

Keywords: Polybenzene, Multi torus, Genus of structure, Linear periodic network, Omega polynomial.

2000 Mathematics subject classification: 05C12

1. Introduction

The polybenzene unit BTA_48 (Figure 1, top, left) was shown [35] to dimerize to three different dimers BTA2_88, BTA2_84 and BTA2_90 , by identifying the rings R(8) and R(12), respectively. Among these, the "eclipsed" dimer BTA2_90, shows suitable angles to form a hyper-pentagon (Figure 1, bottom, left) structures of five-fold symmetry, eventually called multi-tori. The unit BTZ_24 (Figure 1, top, right) can form only an "eclipsed" dimer BTZ2_48

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which of course can form a hyper-pentagon (Figure 1, bottom, right) and next multi-tori.

Multi-tori are complex structures consisting of more than one single torus [4,13,14]. They include negatively curved substructures [24,25,37], termed schwarzites, in the honor of H. A. Schwarz [29,30], who firstly investigated the differential geometry of this kind of surfaces. Multi tori can appear as self-assembly products of some repeating units/monomers, formed by spanning of cages/fullerenes, as in the case of spongy carbon or in natural zeolites. Multi tori MT can grow by a linear periodicity or by forming spherical arrays of various complexity [13]. They can be designed by appropriate map operations [3,5,11,15,33], as implemented in our original software CVNET [34] and Nano Studio [27].

The name of multi tori, bearing the benzene patch, will have B as a prefix. Next, because the opening faces show either "zig-zag" or "armchair" endings, "Z" or "A" will be added as a suffix to their name, as in BTZ or BTA. The number of repeating units and/or number of atoms will be added after the letters.

The design of simple units used to build up multi-tori was made by using some operations on maps, applied on the Tetrahedron T (see the letter "T" in the name of these units).

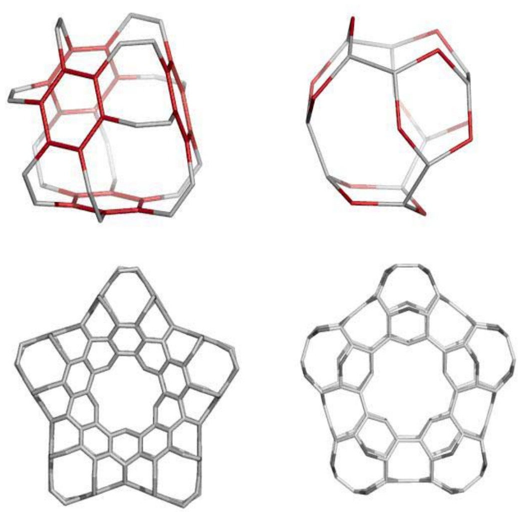

FIGURE 1. BTA_48 and BTZ_24 units and their corresponding hyper-pentagons $BTX_{Cy}5$.

2. Design of Multi Tori

The hyper-ring $BTX_{Cy}5$, (X=A, Z, Figure 1, bottom), can self-arrange to a spherical multi torus BTX20 (Figure 2, left column), of genus g=21, with a well-defined core: -f_5($Le_{2,2}$(Do))=core(BMTA20)_180, while -d_5(S_2(Ico)=core (BMTZ20)_120. In the above, -f_5 means deletion of all pentagonal faces in the transformed by Leapfrog (2,2) of the Dodecahedron Do, and d_5 is deletion of vertices of degree d=5, in the transform of Icosahedron=Ico by the septupling S_2 operation. Also, -d_5(S_2(Ico)=Op(Le(Ico)).

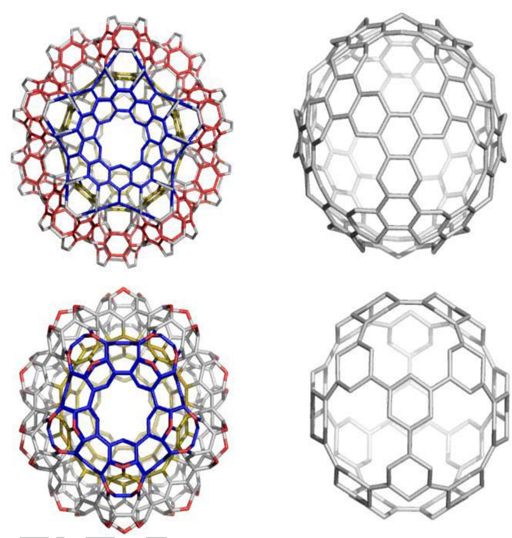

Figure 2. Bottom row: multi torus **BT**A20_1_780 (left) and its core_180 (right) designed by -f_5($Le_{2,2}$(Do)). Top row: multi torus **BTZ**20_1_480 (left) and its core_120 (right) designed by -d_5(S_2(Ico).

A linear array of BTX20, with the repeating unit formed by two units superimposing one pentagonal hyper-face (i.e., $BTX_{Cy}5$), rotated to each other by an angle of PI/5 as in the "dimer" BTX20_2 (X=A, Figure 3, left). Next, the structure can evolve with a one-dimensional periodicity, as shown in BTX20_4 (Figure 3, right).

The number u of tetrahedral units BTX in the linear array of BTX20_k (Table 1) is u=20k-5(k-1)=15k+5, according to the construction mode. The term -5(k-1) accounts for the superimposed hyper-rings $BTX_{Cy}5$, k being the number of units BTX20.

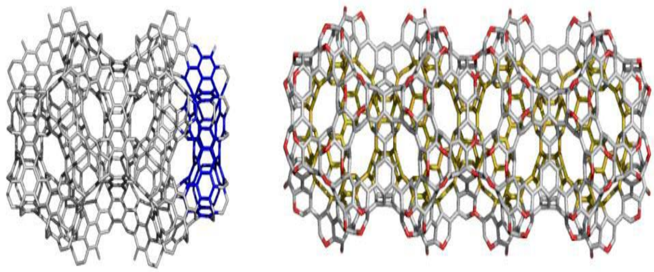

FIGURE 3. The repeating unit BTA20_2_1350 (left) and a rod-like array BTZ20_4_1560 (right).

The number u is also related to the number of faces as: $u = f_8/6$ in case BTA and $u = f_6/4$in case BTZ (see Table 1).

The genus g of the surface where a structural graph is embedded counts the number of simple tori consisting that graph [20].

Theorem. [16,36] *In multi tori built up from open tetrahedral units, the genus of structure equals the number of its units plus one, irrespective of the unit tessellation.*

Demonstration comes out from construction: there are five tetrapodal units to be inserted into exactly five simple tori and all-together are joined to the central torus (see Figure 1, bottom), thus demonstrating the first part of the theorem.

For the second part, we apply the Euler's theorem [18]: $v - e + f = 2(1 - g)$, where $v = |V(G)|$ is the number of vertices/atoms, $e = |E(G)|$, the number of edges/bonds and f is the number of faces of the graph/molecule. Data in Table 1 provide the values of g in several BTX multi tori, tessellation differing as X=A or Z, thus completing the demonstration

Table 1. Euler formula calculation in multi tori BTX.

	BTX	v	e	f_6	f_8	f_{tot}	2(1-g)	g	u	u-formula
1	BTACy5	210	285	35	30	65	-10	6	5	$f_8/6$
2	BTZCy5	120	165	20	15	35	-10	6	5	$f_6/4$
3	BTA20_1	780	1110	170	120	290	-40	21	20	$f_8/6$
4	BTZ20_1	480	690	80	90	170	-40	21	20	$f_6/4$
5	BTA20_5	3060	4410	710	480	1190	-160	81	80	$f_8/6$
6	BTZ20_5	1920	2790	320	390	710	-160	81	80	$f_6/4$

3. Omega Polynomial in **Linear Multi Tori BT**X20_k

In a connected graph $G(V,E)$, with the vertex set $V(G)$ and edge set $E(G)$, two edges $e = uv$ and $f = xy$ of G are called *codistant* e *co* f if they obey the relation [22]:

$$d(v,x) = d(v,y) + 1 = d(u,x) + 1 = d(u,y) \tag{1}$$

which is reflexive, that is, e *co* e holds for any edge e of G, and symmetric, if e *co* f then f *co* e. In general, relation *co* is not transitive; if "*co*" is also transitive, thus it is an equivalence relation, then G is called a *co-graph* and the set of edges $C(e) := \{f \in E(G);\ f \ co\ e\}$ is called an *orthogonal cut oc* of G, $E(G)$ being the union of disjoint orthogonal cuts: $E(G) = C_1 \cup C_2 \cup ... \cup C_k$, $C_i \cap C_j = \emptyset$, $i \neq j$. Klavzar [23] has shown that relation *co* is a theta Djokovi-Winkler relation [17,39].

We say that edges e and f of a plane graph G are in relation *opposite, e op f,* if they are opposite edges of an inner face of G. Note that the relation *co* is defined in the whole graph while *op* is defined only in faces. Using the relation *op* we can partition the edge set of G into *opposite* edge *strips, ops.* An *ops* is a quasi-orthogonal cut *qoc*, since *ops* is not transitive.

Let G be a connected graph and $S_1, S_2, ..., S_k$ be the *ops* strips of G. Then the *ops* strips form a partition of *E(G)*. The length of *ops* is taken as maximum. It depends on the size of the maximum fold face/ring $\mathrm{F}_{max}/\mathrm{R}_{max}$ considered, so that any result on Omega polynomial will have this specification.
Denote by $m(G,s)$ the number of *ops* of length s and define the Omega polynomial as [1,6-10,12,28,38]:

$$\Omega(G,x) = \sum_s m(G,s) \cdot x^s \tag{2}$$

Its first derivative (in x=1) equals the number of edges in the graph:

$$\Omega'(G,1) = \sum_s m(G,s) \cdot s = e = |E(G)| \tag{3}$$

On Omega polynomial, the Cluj-Ilmenau index [26], CI=$CI(G)$, was defined:

$$CI(G) = \{[\Omega'(G,1)]^2 - [\Omega'(G,1) + \Omega''(G,1)]\} \tag{4}$$

Formulas to calculate Omega polynomial and CI index in the two infinite networks BTA20k and BTZ20k, designed on the ground of BTA_48 and BTZ_24 units, are presented in Tables 2 and 3. Formulas were derived from the numerical data calculated on rods consisting of k units BTX20. Omega polynomial was calculated at R_{max}=R(8); examples are given in view of an easy verification of the general formulas. Formulas for the number of atoms, edges and rings (R_6, R_8 and R_{15}, the last one being the simple ring of the hyper-ring $\mathrm{BTX}_{Cy}5$), are included in Tables 2 and 3. Note the Omega polynomial description is an alternative to the crystallographic description.

Table 2. Formulas for Omega polynomial and net parameters in linear periodic BTA20_k network.

BMTA20_k	$\mathrm{R}_{max}(8)$; $\Omega(BMTA20\_k\_R_8) = 10(k+2)X^3 + 5(k-1)X^4 + (11k+1)X^5 + 20(k+3)X^8 + 10(k-1)X^{10} + 15(k-1)X^{12} + (11k+1)X^{20} + 10X^{2(3k+1)}$ $\Omega'(1) = 825k + 285 = \|E(G)\| = edges$; $CI(G) = 15(45351k^2 + 30715k + 5332)$; $atoms = 10(57k+21) = \|V(G)\|$; $R_6 = 5(27k+7)$; $R_8 = 30(3k+1)$; $R_{15} = 11k+1$; $u_{48} = 20k - 5(k-1) = 5(3k+1) = R_8/6$; $g = 1 + u_{48}$
Examples	k=5; CI=19390230; atoms=3060; edges=4410; R_6=710; R_8=480; R_{15}=56; u_{48}=80; g=81. k=6; CI=27333870; atoms=3630; edges=5235; R_6=845; R_8=570; R_{15}=67; u_{48}=95; g=96.

Table 3. Formulas for Omega polynomial and net parameters in linear periodic BTZ20_k network.

BMTZ20_k	$\mathrm{R}_{max}(8)$ $\Omega(BMTZ20\_k\_R_8) = 10(k+2)X^2 + 30kX^3 + (11k+1)X^5 + 10(k+5)X^6 + 10(k-1)X^8 + 10(k-1)X^{10} + 6kX^{20}$ $\Omega'(1) = 525k + 165 = \|E(G)\| = edges$ $CI(G) = 5(55125k^2 + 33653k + 5392)$ $atoms = 120(3k+1) = \|V(G)\| = 24u_{24} = 6R_6$ $R_6 = 20(3k+1) = \|V(G)\|/6$; $R_8 = 15(5k+1)$; $R_{15} = 11k+1$ $u_{24} = 20k - 5(k-1) = 5(3k+1) = R_6/4$; $g = 1 + u_{24}$
Examples	k=5; $70\mathrm{X}^2+150\mathrm{X}^3+56\mathrm{X}^5+100\mathrm{X}^6+40\mathrm{X}^8+40\mathrm{X}^{10}+30\mathrm{X}^{20}$ CI=7758910; atoms=1920; edges=2790; R_6= 320; R_8=390; R_{15}=56; u_{24}=80; g=81. k=6; $80\mathrm{X}^2+180\mathrm{X}^3+67\mathrm{X}^5+110\mathrm{X}^6+50\mathrm{X}^8+50\mathrm{X}^{10}+36\mathrm{X}^{20}$ CI=10959050; atoms=2280; edges=3315; R_6=380; R_8=465; R_{15}=67; u_{24}=95; g=96.

4. Conclusions

Polybenzene units BTX_48 was shown to dimerize forming "eclipsed" isomers, the oligomers of which form structures of five-fold symmetry, called multi-tori.

Multi-tori can grow by a linear periodicity or by forming spherical arrays of various complexity [2]. They can be designed by appropriate map operations [10-14], as implemented in the software CVNET [15] and Nano Studio [16] developed at TOPO Group Cluj. The genus of multi-tori was calculated from the number of tetrapodal units they consist. A description, in terms of Omega polynomial, of the two linear BTX-networks was also presented. We mention that in the last years several authors have published articles dealing with the calculation of various topological indices [2,21,26,32] and counting polynomials [19,31].

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