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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 S₂ 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 $-f_5(Le_{2,2}(\text{Do}))$. Top row: multi torus **BTZ20_1_480** (left) and its core_120 (right) designed by $-d_5(S_2(\text{Ico}))$.

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

	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	$f_{6}/4$

Table 1. Euler formula calculation in multi tori BTX.

3. Omega Polynomial in Linear Multi Tori BTX20_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]:

$$d(v,x) = d(v,y) + 1 = d(u,x) + 1 = d(u,y)$$
(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: $E(G) = C_1 \cup C_2 \cup \ldots \cup C_k, \ C_i \cap C_j = \emptyset, \ i \neq j$. 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 F_{max}/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]:

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

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

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

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

$$CI(G) = \{ [\Omega'(G,1)]^2 - [\Omega'(G,1) + \Omega''(G,1)] \}$$
(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 (R₆, R₈ and R₁₅, the last one being the simple ring of the hyper-ring 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	$\mathbf{R}_{max}(8);$						
	$\Omega(BMTA20_k_R) = 10(k+2)X^3 + 5(k-1)X^4 + (11k+1)X^5 + 20(k+3)X^8 +$						
	$10(k-1)X^{10} + 15(k-1)X^{12} + (11k+1)X^{20} + 10X^{2(3k+1)}$						
	$\Omega'(1) = 825k + 285 = E(G) = edges;$						
	$CI(G) = 15(45351k^2 + 30715k + 5332);$						
	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;						
	$\label{eq:CI27333870; atoms=3630; edges=5235; R_6=845; R_8=570; R_{15}=67; u_{48}=95; g=96.$						

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

BMTZ20_k	$ \begin{split} & \mathbf{R}_{max}(8) \\ & \Omega(BMTZ20_k \mathbf{-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} \end{split} $
Examples	$k=5; 70X^{2}+150X^{3}+56X^{5}+100X^{6}+40X^{8}+40X^{10}+30X^{20}$
	$\label{eq:ci} CI=7758910; \ atoms=1920; \ edges=2790; \ R_6=320; \ R_8=390; \ R_{15}=56; \ u_{24}=80; \ g=81.$
	$k=6; 80X^{2}+180X^{3}+67X^{5}+110X^{6}+50X^{8}+50X^{10}+36X^{20}$
	$CI=10959050; \ atoms=2280; \ edges=3315; \ R_6=380; \ R_8=465; \ R_{15}=67; \ u_{24}=95; \ g=96.$

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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