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ORIGINAL PAPER

Omega polynomial in twisted/chiral polyhex tori

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Abstract The newly proposed Omega counting polynomial is investigated in case of twisted/chiral polyhex tori. Basic definition and properties are given. A factorization procedure is proposed for finding analytical relationships in families of polyhex toroidal nanostructures. Numerical data are also given.

Keywords Omega polynomial · Chiral polyhex tori · Polynomial factorization

1 Introduction to counting polynomials

Among several representations of a graph we mention: a connection table, a sequence of numbers, a matrix, a polynomial or a derived number (called a topological index). In Quantum Chemistry, the early Hűckel theory calculates the levels of π-electron energy of the molecular orbitals, in conjugated hydrocarbons, as roots of the *characteristic polynomial* [1,2]:

$$P(G, x) = \det[x\mathbf{I} - \mathbf{A}(G)] \tag{1}$$

In the above, **I** is the unit matrix of a pertinent order and **A** the adjacency matrix of the graph G. The characteristic polynomial is used in evaluating of the topological resonance energy TRE, the topological effect on molecular orbitals TEMO, the aromatic sextet theory, the Kekulé structure count, etc. [1–6].

Dedicated to Professor Haruo Hosoya, Ochanomizu University, Tokyo, Japan, for his bright contribution to Chemical Graph Theory.

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The coefficients $m(G, k)$ in the polynomial expression:

$$P(G, x) = \sum_k m(G, k) \cdot x^k \tag{2}$$

can be calculated from the graph G by a method making use of the Sachs graphs, which are subgraphs of G. Relation (2) was found independently by Sachs, Harary, Milić, Spialter, Hosoya, etc. [1,2]. The above method is useful in small graphs but in larger ones the numeric methods of linear algebra, such as the recursive algorithms of Le Verier, Frame, or Fadeev, are more efficient [7,8].

An extension of relation (1) was made by Hosoya [9] and others [10–14] by changing the adjacency matrix with the distance matrix and next by any square topological matrix.

Relation (2) is a general expression of a counting polynomial, written as a sequence of numbers, with the exponents showing the extent of partitions $p(G), \cup p(G) = P(G)$ of a graph property $P(G)$ while the coefficients $m(G, k)$ are related to the occurrence of partitions of extent k.

Counting polynomials have been introduced, in the Mathematical Chemistry literature, by Hosoya [15,16].

Some distance-related properties can be expressed in the polynomial form, with coefficients calculable from the layer and shell matrices [17–20].

2 Omega polynomial

Omega polynomial [21] $\Omega(G, x)$ counts the orthogonal edge-cuts in a polygonal lattice. Let $G(V, E)$ be a connected bipartite graph. Two edges $e = (1, 2)$ and $e' = (1', 2')$ of G are called codistant (briefly: e co e') if for $k = 0, 1, 2, \ldots$ there exist the relations: $\mathrm{d}(1, 1') = \mathrm{d}(2, 2') = k$ and $\mathrm{d}(1, 2') = \mathrm{d}(2, 1') = k+1$ or vice versa. For some edges of a connected graph G there are the following relations satisfied [22,23]:

$$e\ co\ e \tag{3}$$

$$e\ co\ e' \Leftrightarrow e'\ co\ e \tag{4}$$

$$e\ co\ e' \,\&\, e'\ co\ e'' \Rightarrow e\ co\ e'' \tag{5}$$

though relation (5) is not always valid.

Let $C(e) := \{e' \in E(G); e'\ co\ e\}$ denote the set of all edges of G which are codistant to the edge e. If all the elements of $C(e)$ satisfy the relations (3–5) then $C(e)$ is called an *orthogonal cut* "*oc*" of the graph G. The graph G is called *co-graph* if and only if the edge set $E(G)$ is the union of disjoint orthogonal cuts: $C_1 \cup C_2 \cup \ldots \cup C_k = E$ and $C_i \cap C_j = \emptyset$ for $i \neq j$, $i, j = 1, 2, \ldots, k$.

If any two edges of an edge-cut sequence are codistant (obeying the relations (3) and (4)) and *belong to one and the same face* of the covering, such a sequence is called

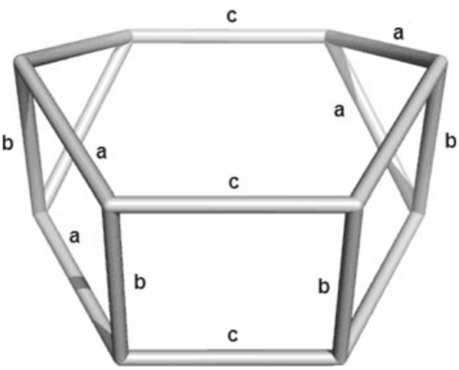

Fig. 1 The *"qoc"* strips and Omega polynomial of a polyhedral cage: $\Omega(G,x) = x^3 + 3x^4$; $CI = 168$; $I_\Omega = 1.91109$

a *quasi-orthogonal cut "qoc"* strip. This means that the transitivity relation (5) is not necessarily obeyed. An example is given in Fig. 1.

A *qoc* strip starts and ends either out of G (at an edge with endpoints of degree lower than 3, if G is an open lattice,) or in the same starting polygon (if G is a closed lattice). Any *oc* strip is a *qoc* strip but the reverse is not always true [24,25].

The term "co-distant" is synonym (in some extent) with "equidistant" or "topologically parallel".

3 Twisted/chiral tori of T(6, 3)VV$t[c, n]$ family

The attention was focused to the chiral/twisted T(6, 3)VV$t[c, n]$ objects, because they offer cases of single term Omega polynomials, with direct interpretation of their spirality. We present here a *factorization* procedure enabling the derivation of formulas for a whole family of chiral polyhex toroids.

Within the present *factorization* procedure, [26,27] the Omega polynomial of a torus T is written, cf. (6), as the product:

$$\Omega(T,x) = f_{k/k_i} \cdot \Omega(T_{i,x}) = \sum_{c_i} f_{k/k_i} \cdot m(T_{i,c_i}) \cdot x^{f_{k/k_i} \cdot c_i} \tag{6}$$

In the above relation, k is the *size* factor multiplying the net ratio $r = c/n$ to give the actual size $s : s = r \cdot k$. Next, k_i refers to the divisors of k and, correspondingly, T_i and c_i refer to the object showing the k_i size factor. Finally, f_{k/k_i} is the factor to be used in the actual procedure.

Case: T(6, 3) VV$t[c, n]$. The chosen class shows a net ratio $(c/n) = (4/6)$ and the size factor is: $k = c/4 = n/6$. Next, $c = kc_1$; $n = kn_1$, with $c_1 = 4$ and $n_1 = 6$ being the net dimensions of the first (smallest) family of objects in this class . A family of twisted tori includes all the objects having the same $[c, n]$-dimensions (implying the same k) and $0 \leq t \leq c$, in Diudea's system [28]. In the discussed case, the maximum twisting is taken $t = c/2$, to ensure all the objects are distinct [29]. Figure 2 illustrates a torus of this class, which shows a single term Omega polynomial.

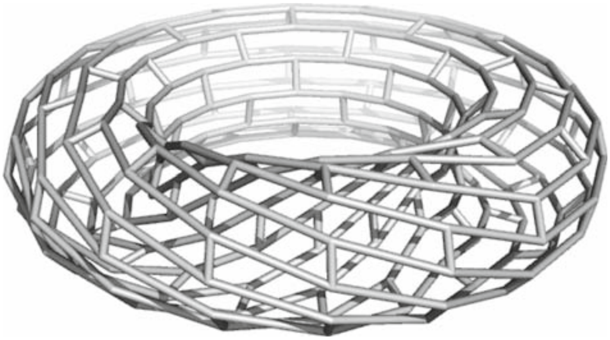

Fig. 2 Torus T(6, 3)VV6[12, 18]; v = 216, with the twisted region in the front (non-optimized)

The procedure to derive formulas for a whole family of chiral polyhex toroids is as follows [27].

Table 1 Formulas for Omega polynomial of T(6, 3)VV$t[c, n]$ polyhex tori; $(c/n) = (4/6) \cdot k$

k	t-mode	s	Omega polynomial
odd	0	–	(a) $c \cdot x^{n/2} + (c/2) \cdot x^{2n}$; non-twisted; non-chiral
			(b) $kc_1 \cdot x^{kn_1/2} + k(c_1/2) \cdot x^{2kn_1}$
			(c) $f_{k/k_i}(c_i) \cdot x^{f_{k/k_i}(n_i/2)} + f_{k/k_i}(c_i/2) \cdot x^{f_{k/k_i}(2n_i)}$
	$4s+2$	$0, 1, 2, \ldots, (c-12/8)$	(a) $n/k \cdot x^{kn}$
			(b) $n_1 \cdot x^{k^2 n_1}$
			(c) $f_{k/k_i}(n_i/k_i) \cdot x^{f_{k/k_i}(k_i n_i)}$
	$4s$	$1, 2, \ldots, (c-4)/8$	(a) $c/k \cdot x^{kn/2} + c/2k \cdot x^{2kn}$
			(b) $c_1 \cdot x^{k^2 n_1/2} + c_1/2 \cdot x^{2k^2 n_1}$
			(c) $f_{k/k_i}(c_i/k_i) \cdot x^{f_{k/k_i}(k_i n_i/2)} + f_{k/k_i}(c_i/2k_i) \cdot x^{f_{k/k_i}(2k_i n_i)}$
	$4s+2$	$(c-4)/8$; t $= c/2$	(a) $3t \cdot x^{cn/2t} = n \cdot x^n$
			(b) $kn_1 \cdot x^{kn_1}$
			(c) $f_{k/k_i}(n_i) \cdot x^{f_{k/k_i}(n_i)}$
even	0	–	as for $k =$ odd
	$4s+2$	$0, 1, 2, \ldots, (c-8/8)$	(a) $c/2k \cdot x^{kn} + c/2k \cdot x^{2kn}$
			(b) $c_1/2 \cdot x^{k^2 n_1} + c_1/2 \cdot x^{2k^2 n_1}$
			(c) $f_{k/k_i}(c_i/2k_i) \cdot x^{f_{k/k_i}(k_i n_i)} + f_{k/k_i}(c_i/2k_i) \cdot x^{f_{k/k_i}(2k_i n_i)}$
	$4s$	$c/8$; $t = c/2$	as for $k =$ odd

Table 2 Examples of Omega polynomial and CI index in polyhex tori of T(6, 3)VV$t[c, n]$ series

k; $[c, n]$	t-mode & f_{k/k_i}	s	t	Omega polynomial	CI
k = odd					
1; [4,6]					
	0		0	$4x^3 + 2x^{12}$	972
	4s + 2	0	2; c/2	$6x^6$	1080
3; [12,18]					
	0		0	$12x^9 + 6x^{36}$	96228
	4s + 2	0	2	$6x^{54}$	87480
	4s	1	4	$4x^{27} + 2x^{108}$	78732
	4s + 2	1	6; $c/2$	$18x^{18}$	99144
5; [20,30]					
	0		0	$20x^{15} + 10x^{60}$	769500
	4s + 2	0	2	$6x^{150}$	675000
	4s	1	4	$4x^{75} + 2x^{300}$	607500
	4s + 2	1	6	$6x^{150}$	675000
	4s	2	8	$4x^{75} + 2x^{300}$	607500
	4s + 2	2	10; $c/2$	$30x^{30}$	783000
9; [36,54]					
	0		0	$36x^{27} + 18x^{108}$	8266860
	4s + 2	0	2	$6x^{486}$	7085880
	4n	1	4	$4x^{243} + 2x^{972}$	6377292
	$f_{9/3}$	–	6	$18x^{162}$	8030664
	4s	2	8	$4x^{243} + 2x^{972}$	6377292
	4s + 2	2	10	$6x^{486}$	7085880
	$f_{9/3}$	–	12	$12x^{81} + 6x^{324}$	7794468
	4s + 2	3	14	$6x^{486}$	7085880
	4s	4	16	$4x^{243} + 2x^{972}$	6377292
	4s + 2; $f_{9/3}$	4	18; $c/2$	$54x^{54}$	8345592
k = even					
2; [8,12]					
	0		0	$8x^6 + 4x^{24}$	18144
	4s + 2	0	2	$2x^{24} + 2x^{48}$	14976
	4s	1	4; $c/2$	$12x^{12}$	19008
4; [16,24]					
	0		0	$16x^{12} + 8x^{48}$	311040
	4s + 2	0	2	$2x^{96} + 2x^{192}$	239616
	$f_{4/2}$	–	4	$4x^{48} + 4x^{96}$	285696
	4s + 2	1	6	$2x^{96} + 2x^{192}$	239616
	4s; $f_{4/2}$	2	8; $c/2$	$24x^{24}$	317952

Table 2 continued

k; $[c, n]$	t-mode & f_{k/k_i}	s	t	Omega polynomial	CI
6; [24,36]					
			0	$24x^{18}+12x^{72}$	1609632
	4s + 2	0	2	$2x^{216}+2x^{432}$	1213056
	$f_{6/3}$	–	4	$12x^{108}$	1539648
	$f_{6/2}$	–	6	$6x^{72}+6x^{144}$	1524096
	$f_{6/3}$	–	8	$8x^{54}+4x^{216}$	1469664
	4s + 2	2	10	$2x^{216}+2x^{432}$	1213056
	4s; $f_{6/2}$; $f_{6/3}$		12; $c/2$	$36x^{36}$	1632960

1. If k is *odd*, ($k = 1, 3, \ldots$) and *prime* number, formulas for two sub-series of tori can be written: (a) objects having the twisting $t = 4s + 2$ and (b) objects with $t = 4s$, the limits for s being given in Table 1. The objects of series (a) show a single term in the Omega polynomial while those in the series (b) show a double term polynomial. Formulas for the non-twisted objects are also included. All the formulas in Table 1. are given in three forms: (i) general, non-factorized; (ii) factorized vs. $k_1 = 1$ and (iii) factorized vs. any divisor of k, $k_i = i$.
2. Take a *non-prime* k-value and find its divisors. Factorize first the t-parameter of the divisors and next write the corresponding (distinct) polynomial formulas (by using the factors f_{k/k_i}- see Tables 1 and 2) for all the possible divisors. Complete the actual t-parameter up to $t = c/2$ and use the corresponding formulas for (prime number) odd k objects given in Table 1 Note that the factorizing mode is dominant with respect to the actual twisting t-mode.
3. Write formulas for the *even* series ($k = 2, 4, \ldots$) analogously; remark the only new formula is for $t = 4s + 2$.
4. Calculate the actual Omega polynomial and the corresponding *CI* index.

Remark that the actual factorization procedure can be seen as a numerical fractalization.

The actual procedure starts with $k = 1$ and, recursively, provides formulas for families of $k > 1$. Examples are given in Table 2. Note that, at various t-values within the same t-mode (either 4s+2 or 4s), degenerate polynomial and *CI* values appear.

The remark on spirality refers to the formula $3t \cdot x^{cn/2t} = n \cdot x^n$ for the single term Omega polynomial of the maximum twisted objects of this class. As a hexagon is the start of three edge-cut strips, $t = n/3$ is just the number of spirals of this object. For the other objects, t is more hidden, because of the degeneracy of edge-cut modes (see Table 2).

The toroidal objects were generated by the TORUS [30] while the Omega polynomial was calculated by the OMEGA COUNTER [31] original programs.

4 Conclusions

Counting polynomials represent a class of polynomials, whose coefficients can be calculated either from matrices or by means of orthogonal edge-cuts (as in the discussed case). Basic definitions and properties of the Omega polynomial were given. Analytical formulas for calculating the polynomial in twisted polyhex tori were derived by means of an original factorization procedure. The motivation of this study was the fact that single term Omega polynomials allow direct interpretation of the toroidal spirality.

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