Counting Kekulé Numbers in Torenes
A Conjecture

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Abstract. An algorithm for calculating the number of Kekulé structures of a polyhex torus (in polynomial time) **based on a conjecture** is presented. The algorithm, called B, is given in the very short, therefore the interesting reader find more information (the algorithm A) in ref. 2.

This paper is dedicated to Professor Klaus Möckel (Mühlhausen/Germany)
on his 75th birthday

1. Introduction

Crop circles fullerenes[1] recently discovered in the soot are presumably torus-shaped „graphitoids“. Such structures may be called *toroidal polyhexes* or *torenes*, if all their polygonal faces are hexagons and *toroidal fullerenes*, if their faces are of mixed ring sizes.[2,3] Note that the torus is a closed surface *S* that can carry graphs *G* such that all its vertices have degree 3 and all faces of the embedding of *G* in *S* are hexagons (Figure 1). Pioneering papers on this topic are due to Kirby,[4] Randić *et al*,[5] and John.[6]

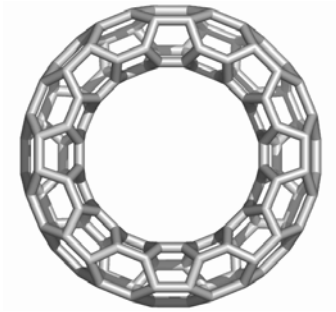

Figure 1: A polyhex torus.

In this paper, an algorithm B for calculatig the number of Kekulé structures of a polyhex torus (in polynomial time) **based on a conjecture** is presented. The algorithm given here is very short, therefore the interesting reader find more informations (especially another algorithm A) in ref. 2.

Let **T** denote the class of all toroidal polyhexes.[2] The graph of $T \in \mathbf{T}$ can be drawn in the plane (equipped with the regular hexagonal lattice L) using the representation of the torus T by a parallelogram P with the usual boundary identification (see Figure 2, *e.g.*, parallelogram $A = A_1, A_1', B_1'', B_1'''$; identify first line $A_1\ B_1'''$ with line $A_1'B_1''$ and second „circle“ $A_1 A_1'$ with „circle“ $B_1'''\ B_1''$).

For every $T \in \mathbf{T}$, three (not necessarily incongruent) representations T_1, T_2, and T_3 of its graph are obtained (Figure 2). For i = 1, 2, 3 there is $T_i = (p_i, q_i, t_i)$, with p_i being the number of hexagons met by s_i, q_i - the number of layers of hexagons parallel to s_i that are covered by P, and t_i (the *torsion*) - the number of edges of L intersected by s_i between A and B_i.

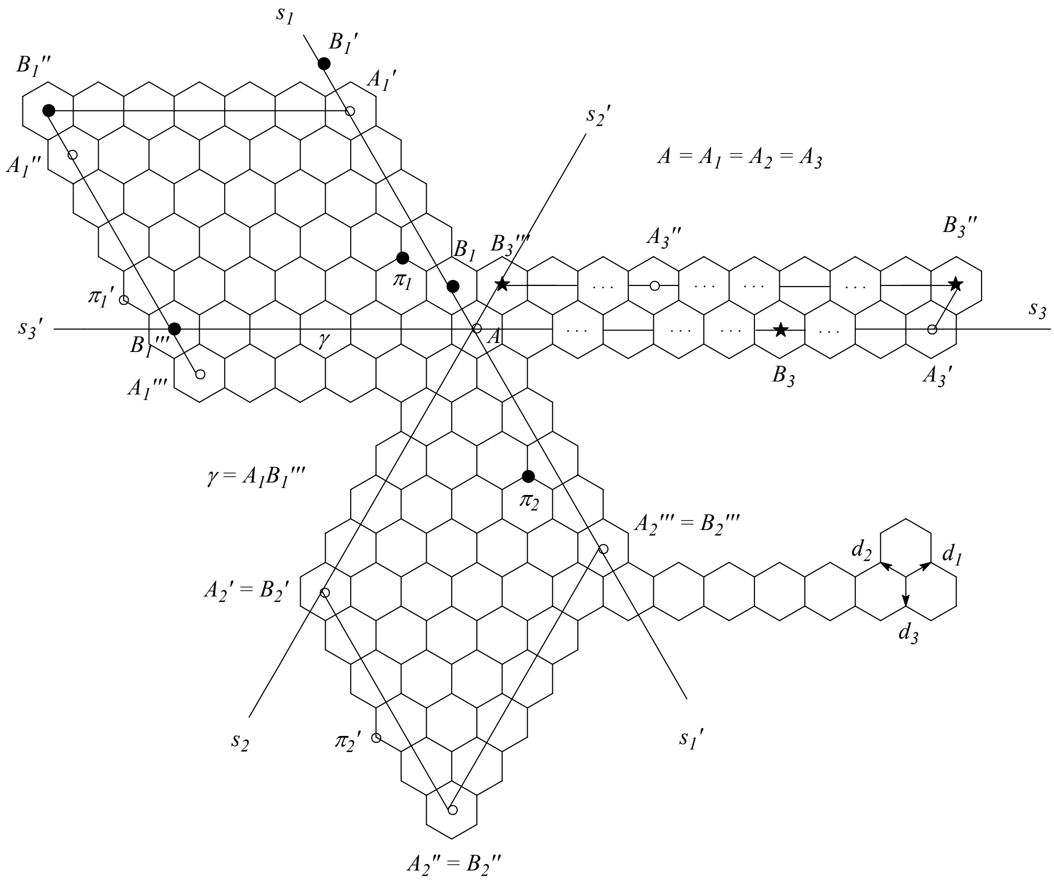

Figure 2: Three representations of a torus T in the regular hexagonal lattice L.

We may assume $p_1 \leq p_2 \leq p_3$. Let $p = p_1$, $q = q_1$, $t = t_1$, $s = s_1$, $T^* = T_1$: then $T^* = T^*(p,q,t)$ is the canonical representation of the graph $T \in \mathbf{T}$. For our example, given in Figure 2, clearly $p = 5$, $q = 6$ and $t = 1$.The parameters p_i, q_i, t_i, $i = 2, 3$, can easily be found using, *e.g.*, the method described in ref. 7.

2. Definitions

Let $G = (V,E)$ be a connected graph with vertex set $V = V(G)$ and edge set $E = E(G)$. Graph G is called *bipartite* if and only if its vertices can be coloured black and white such that every edge connects a white vertex with a black one.

A *matching* M of G is a set of pairwise disjoint edges of G. Matching M is called *perfect* iff M covers all vertices of G . Let $\mathbf{M} = \mathbf{M}(G)$ denote the set of all perfect matchings of G; set $m = m\{G\} = |\mathbf{M}|$. Note that , for $i = 1, 2, 3$, the set of all edges of direction d_i (see Figure 2) is a perfect matching of T.

3. The Algorithm

Assume that T^* has been drawn such that s lies horizontally in the plane (see Figure 3). Graph T^* being bipartite, its vertices can be coloured such that every vertical edge connects a black top vertex with a white bottom vertex. Let $\mathbf{P} = \mathbf{P}(T^*)$ denote the set of all vertical edges of T^* intersected by s ; clearly, $|\mathbf{P}| = p$.

Graph $G(0)$ is obtained from T^* by omitting all edges of $\mathbf{P}$. Clearly, the graph $G(0)$ is the embedding of a planar graph in a cylinder. Note that $m = m\{G(0)\} = 2^q$, see, *e.g.*, ref.[2,8]

For $T \in \mathbf{T}$ we shall now determine the number $m = m\{T\} = h(p,q,t)$.

First we define a p x p *circulant matrix*[9] $\mathbf{S}_1 = circ(0,1,...,0,0)$ and a p x p *skew circulant* matrix $\mathbf{S}_2 = scirc(0,1,...,0,0)$. Matrix $\mathbf{I} = circ(1,0,...0,0) = scirc(1,0,...0,0)$ denote the p x p *unit matrix*.

3.1. Algorithm B

Let $\lambda = 1, 2$.

(**B**.1) **Calculate matrices:**

$$\mathbf{W}_\lambda = \mathbf{W}_\lambda\{G(0)\} = \mathbf{W}_\lambda(p,q,0) = (\mathbf{I} + \mathbf{S}_\lambda)^q \qquad (1)$$

(**B**.2) **Define polynomials:**

$$f_\lambda(T;x) := \det\left(x(\mathbf{S}_\lambda)^t + \mathbf{W}_\lambda\right) \tag{2}$$

(**B**.3) **For** μ = 1,2 **calculate numbers**:

$$g(T;\lambda,\mu) = 1/2\left|f_\lambda(T;1) - (-1)^\mu f_\lambda(T;-1)\right| \tag{3}$$

(**B**.4) **Conjecture** :

$$m(T) = h(p,q,t) = \begin{cases} g(T;1,1) + g(T;2,2) & \text{if } p \text{ is } odd \\ g(T;1,2) + g(T;2,1) & \text{if } p \text{ is } even \end{cases} \tag{4}$$

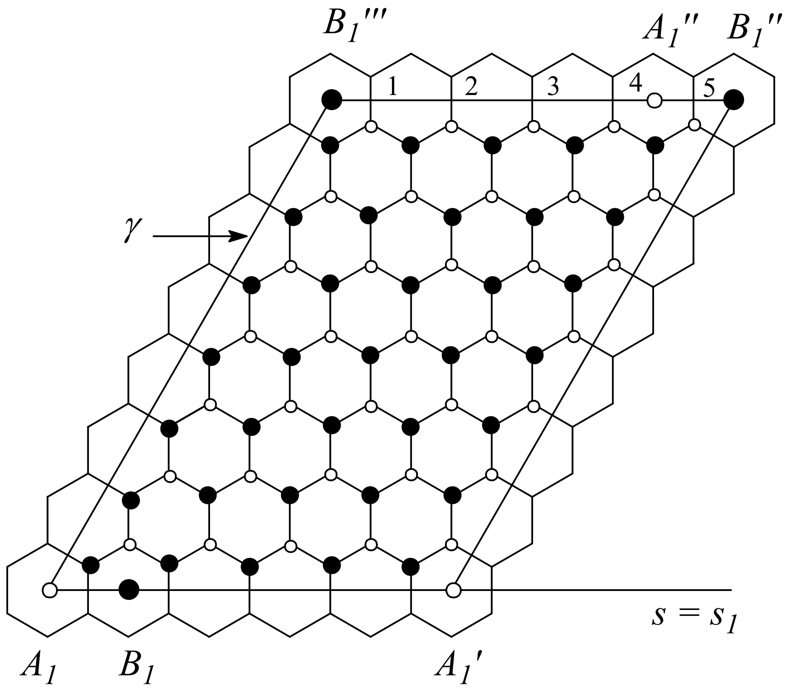

Figure 3: Representation of $T^* = T_1(5,6,1)$, s = s_1 lies horizontally.

3.2. Example

Torene graph T , given in Figure 2, has three different representations $T^*= T_1$, T_2, and T_3. We calculate the number of Kekule' structures for $T^*= T_1= T(5,6,1)$ (p is *odd*) and for $T_2=T(6,5,0)$ (p is *even*).

(a) For $T = T(5,6,1)$ are

$$\mathbf{W}_1 = \mathbf{W}_1(5,6,1) = circ(\mathbf{I} + \mathbf{S}_1)^6 = circ(7,7,15,20,15) \tag{5}$$

and

$$\mathbf{W}_2 = \mathbf{W}_2(5,6,1) = scirc(\mathbf{I} + \mathbf{S}_2)^6 = scirc(-5,5,15,20,15) \tag{6}$$

The polynomials of (**B**.2) are for $T = T(5,6,1)$:

$$f_1(T;x) = x^5 + 35x^4 - 1535x^3 + 20555x^2 + 705x + 64 \tag{7}$$

and

$$f_2(T;x) = -x^5 - 25x^4 - 2125x^3 + 9375x^2 - 15625x \tag{8}$$

Because of p is *odd*, calculate by (**B**.3):

$$g(T;1,1) = 35 + 20555 + 64 = 20654 \tag{9}$$

$$g(T;2,2) = 1 + 2125 + 15625 = 17751 \tag{10}$$

and finally by (**B**.4) is

$$m\{T\} = m\{T(5,6,1)\} = h(5,6,1) = 38405 \tag{11}$$

(b) For $T = T(6,5,0)$ are

$$\mathbf{W}_1 = \mathbf{W}_1(5,6,0) = circ(\mathbf{I} + \mathbf{S}_1)^5 = circ(1,5,10,10,5,1) \tag{12}$$

$$\mathbf{W}_2 = \mathbf{W}_2(6,5,0) = circ(\mathbf{I} + \mathbf{S}_2)^5 = scirc(1,5,10,10,5,1) \tag{13}$$

The polynomials of (**B**.2) are for $T = T(6,5,0)$:

$$f_1(T;x) = x^6 + 6x^5 - 615x^4 + 7160x^3 + 7155x^2 + 7776x \tag{14}$$

and

$$f_2(T;x) = x^6 + 6x^5 + 645x^4 - 5300x^3 + 22785x^2 + 1656x + 32 \tag{15}$$

Because of *p* is *even*, calculate by (**B**.3):

$$g(T;1,2) = 6 + 7160 + 7776 = 14942 \quad (16)$$

$$g(T;2,1) = 1 + 645 + 22785 + 32 = 23463 \quad (17)$$

and finally by (**B**.4) is

$$m\{T\} = m\{T(6,5,0)\} = h(6,5,0) = 38405 = m\{T(5,6,1)\} \quad (18)$$

The polynomials and values for torene T(5,6,*t*), *t* = 0, 2, 3, 4 , are given in the Appendix of this paper.

3.3. Remarks

(1) Note that matrix $\mathbf{W}_\lambda$ is identical with matrix $\mathbf{W}_\lambda$ (0) given in ref.[2] The reader can therein find an example for $T = T(5,6,1)$, the calculation of matrix $\mathbf{W}_\lambda = \mathbf{W}_\lambda(0)$ being made by using of Algoritm **A** (see Figure 4), described in ref. 2.

Explicite formulas for elements of $\mathbf{W}_\lambda$ are given in Remark (3) of that paper.

(2) It is simple to see that for integer *j*:

$$h(p,q,t) = h(p,q,q-t) = h(p,q,t+jp) \quad (19)$$

(3) For natural numbers *n*, $s \geq 0$ and integer *r* define numbers:

$$\begin{bmatrix} n \\ r \end{bmatrix}_s := \sum_k \binom{n}{r+ks}, \quad \begin{Bmatrix} n \\ r \end{Bmatrix}_s := \sum_k (-1)^k \binom{n}{r+ks}$$

where integer *k* satisfies the condition: $-\frac{r}{s} \leq k \leq \frac{n-r}{s}$

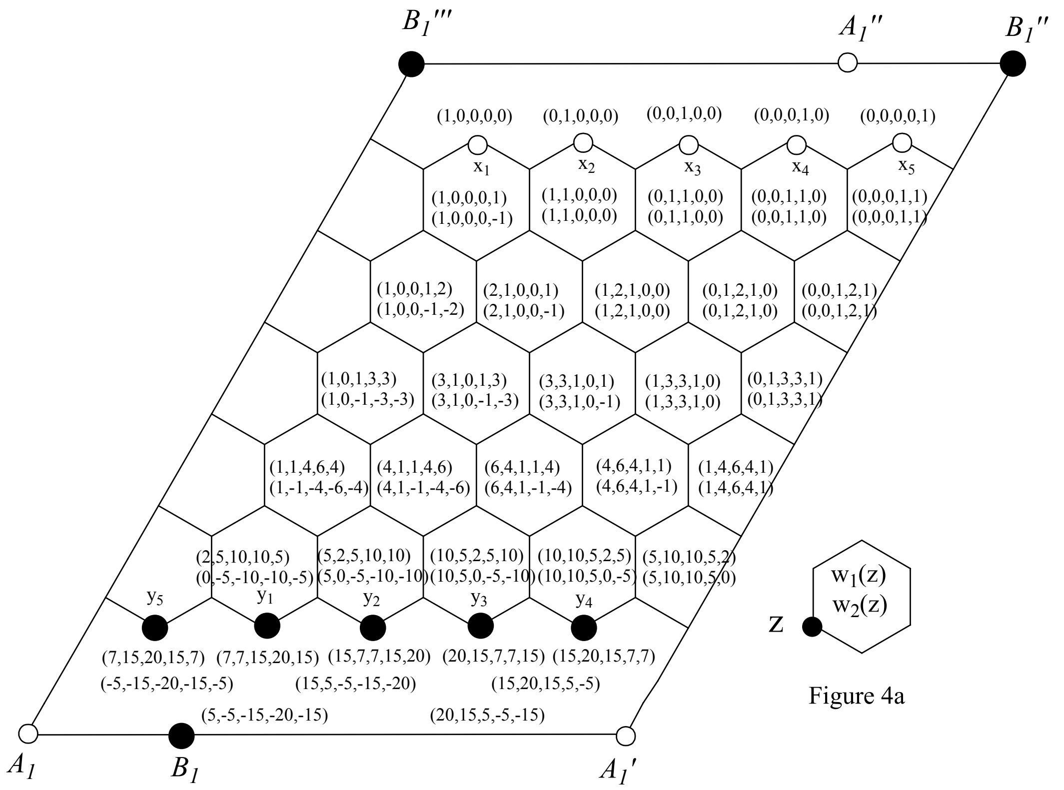

Figure 4: The entries are arranged as indicated in Fig. 4a.

For λ = 1,2 the matrices $\mathbf{W}_\lambda$ we can represent as $\mathbf{W}_1 = circ(c_0, c_1,...,c_{p-1})$ and $\mathbf{W}_2 = scirc(s_0,s_1,...,s_{p-1})$. It is simple to prove by induction over q , that for i = 0, 1, 2, ..., p-1,

$$c_i = c_i(p,q,0) = \begin{bmatrix} q \\ i \end{bmatrix}_p \qquad \text{and} \qquad s_i = s_i(p,q,0) = \begin{Bmatrix} q \\ i \end{Bmatrix}_p$$

Some interesting properties of these *cyclic binomial numbers* will be discussed elsewhere.

4. Appendix

For the remaining t = 0,2,3,4 are the coefficients of $f_\lambda(T;x)$ polynomials:

t	$\lambda = 1$	$\lambda = 2$
0	1; -35; -1535; -20555; 705; -64	1; 35; 2125; - 9375; 15625; 0
2, 4	1; 75; 1025; 20515; -1855; 64	1; 75; 2125; - 3125; 15625; 0
3	1; 100; 2630; 20900; 2305; 64	-1; -100; -2750; -12500; -15625; 0

The $g(T;\lambda,\mu)$ and $m(T) = h(5,6,t)$ values are:

t	$g(T; 1, 1)$	$g(T; 2, 2)$
0; 2; 4	20654	17751
3	21064	18376

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