CROATICA CHEMICA ACTA CCACAA **71** (3) 435–447 (1998)

ISSN-0011-1643
CCA-2503

Original Scientific Paper

Kekulé Count in Toroidal Hexagonal Carbon Cages

Peter E. John

Technical University Ilmenau, Institute of Mathematics, PSF 100565, D–98684 Ilmenau, Germany

Received March 31, 1998; revised July 20; 1998, accepted July 20, 1998

After the fullerenes have been found, it is a natural question to ask whether there are torus-shaped »graphitoid« carbon molecules which may be called *toroidal graphitoids.* Note that the torus is the only closed surface S that can carry graphs G such that all vetices of G have degree 3 and all faces of the embedding of G in S are hexagons (Figure 1). In what follows, such (hypothetical) molecules (see Ref. 1a) and their molecular graphs will be referred to as »*torenes*«.

Note that the first paper about this topic was given by M. Randić, Y. Tsukano, and H. Hosoya.[1b]

In this paper, an algorithm is given that enables the number of Kekulé structures of a torene to be calculated in polynomial time (the complexity problem will be discussed elsewhere).

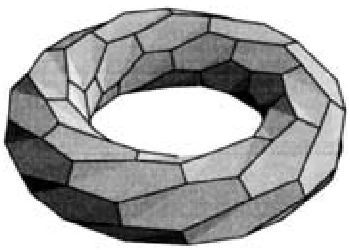


Figure 1

TOROIDAL HEXAGONAL TESSELLATIONS (TORENES)

Let $\mathbf{T}$ denote the class of all torenes. For $T \in \mathbf{T}$ let $h = h(T)$, $v = v(T)$ and $e = e(T)$ denote the numbers of hexagons, vetices and edges of T, respectively. Clearly, $v = 2h$ and $e = 3h$. 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 $A = A_1, A'_1, B''_1, B'''_1$ – note that the points π_1, π'_1, π_2 and π'_2 represent the same point of T). Let d_i (i = 1,2,3) be the edge directions of L (Figure 2).

Select $P = P_i$ such that its sides s_i, s'_{i-1} are perpendicular to d_i, d_{i-1}, respectively, (the subscript i–1 is to be reduced to the smallest positive integer modulo 3). Let p_i and q_i denote the number of hexagons met by s_i, and the number of layers of hexagons parallel to s_i that are covered by P, respectively, and let t_i (the *torsion*) denote the number of edges of L intersected by s_i between A and B_i. In this way, for every $T \in \mathbf{T}$, three (not necessarily incongruent) representations T_1, T_2, T_3 of its graph are obtained.

W.l.o.g. we may assume $p_1 \le p_2 \le p_3$. Let $p = p_1$, $q = q_1$, $t = t_1$, $s = s_1$, $T^* = T_1$: then T^* and p, q, t may be considered the canonical representation, and the canonical parameters, of the graph $T \in \mathbf{T}$, respectively. We shall briefly write $T^* = (p, q, t)$. Note that, for fixed p, q, t, all torenes T' with parameters p, q, t' where $t' \equiv t$ (*mod p*) have the same canonical representation $T^* = (p, q, t)$. For our example given in Figure 2, clearly $p = 5$, $q = 6$ and $t = 1$. The canonical parameters can easily be found using, *e.g.*, the method described in Ref. 2.

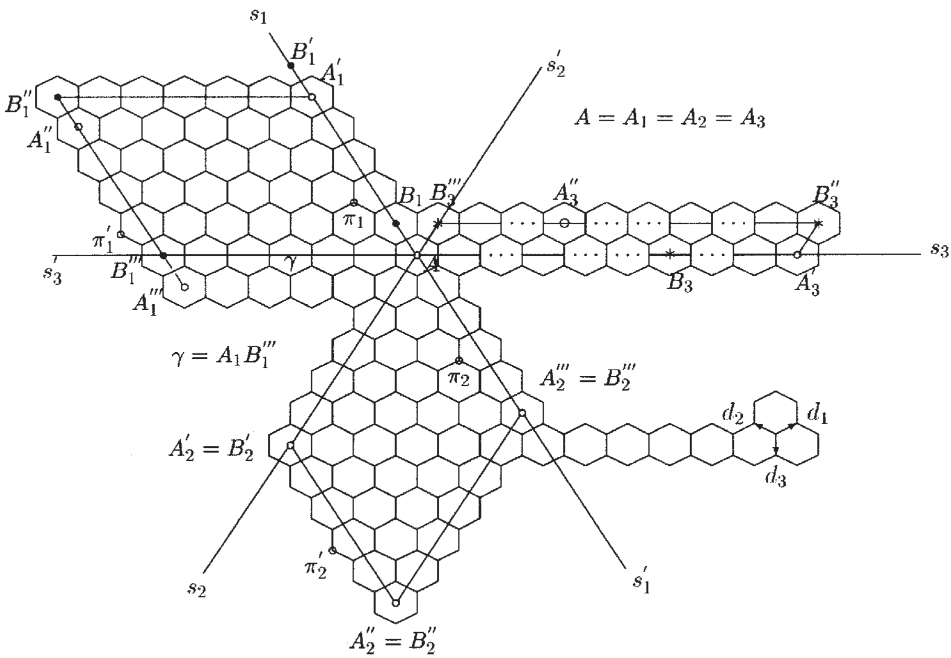


Figure 2

DEFINITIONS

Let $G = (V, E)$ be a connected graph with vertex set $V = V(G)$ and edge set $E = E(G)$. For G, $v = v(G) = |V|$ and $e = e(G) = |E|$ denote the number of vertices and the number of edges of G respectively.

G is called *bipartite* iff its vertices can be coloured white and black 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 $m = m(G) = |\mathbf{M}|$. Let $M \in \mathbf{M}$. The edges of G that belong (do not belong) to M are referred to as the red (blue) edges. The number of perfect matchings of G that contain (do not contain) a given edge $k \in E$ is denoted by $r(G, k)$ ($b(G, k)$): thus $r(G, k) + b(G, k) = m(G)$ for every edge $k \in E$.

Note that, for $i \in \{1,2,3\}$, the set of all edges of direction d_i is a perfect matching of T.

PRELIMINARIES

Assume that T^* has been drawn such that s lies horizontally in the plane (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, $|\mathbf{P}| = p$. Consider the 2^p subsets $\mathbf{R}$ of $\mathbf{P}$ where $|\mathbf{R}| = r \in \{0,1,\ldots,p\}$. Set $\mathbf{B} = \mathbf{P}–\mathbf{R}$.

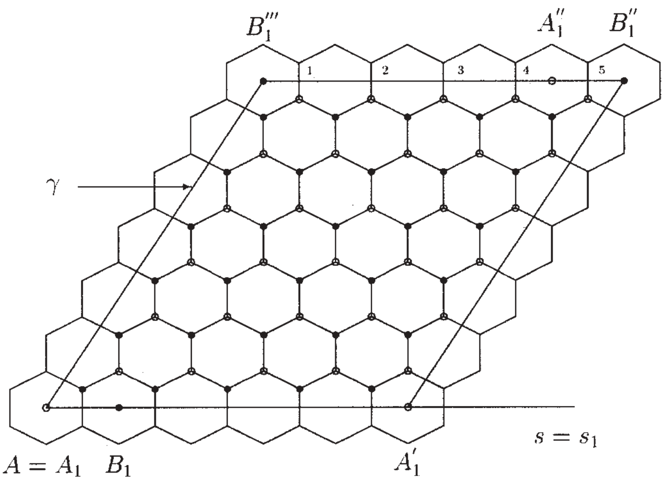


Figure 3

Let $\mathbf{M}(\mathbf{R})$ denote the set of perfect matchings of T that contain all edges of $\mathbf{R}$ but no edge of $\mathbf{B}$ (note that $\mathbf{M}(\mathbf{R})$ may be empty).

$$\mathbf{M}(T) = \bigcup_{\mathbf{R} \subseteq \mathbf{P}} \mathbf{M}(\mathbf{R}) \, . \tag{1}$$

Set

$$m(\mathbf{R}) = \left|\mathbf{M}(\mathbf{R})\right| \, . \tag{2}$$

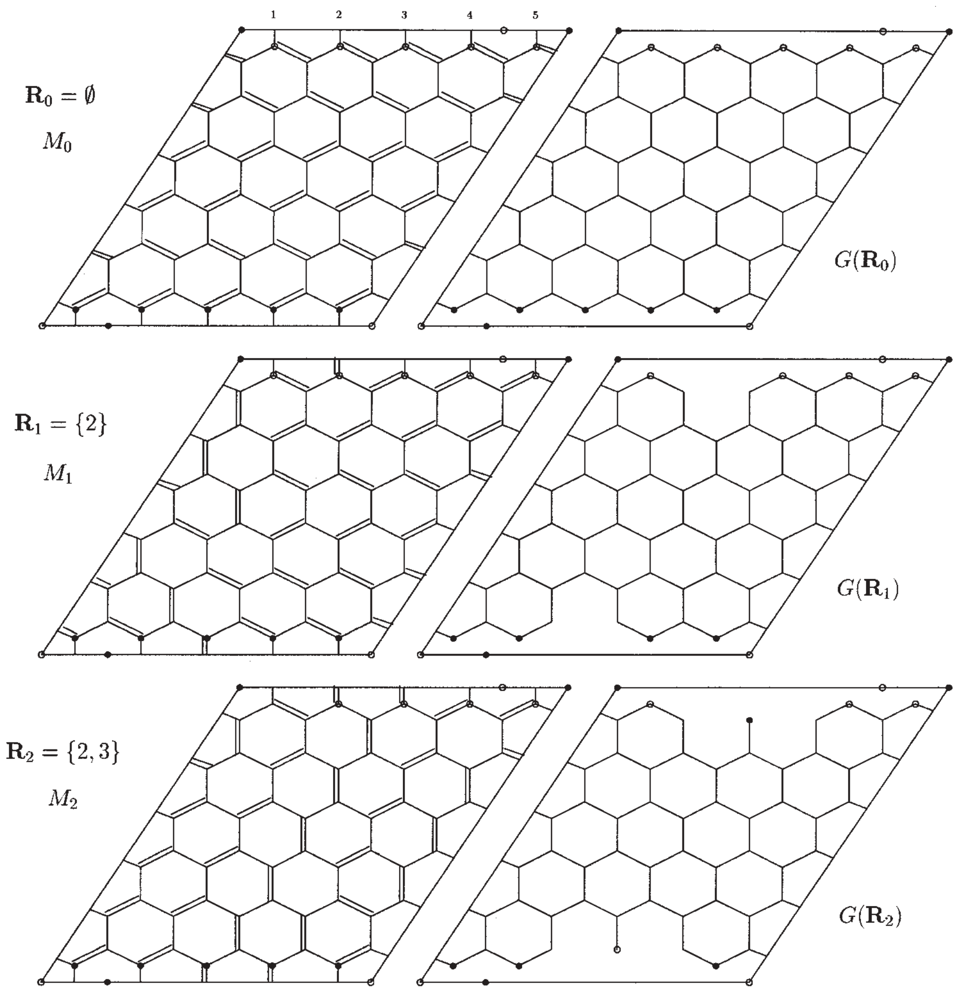


Figure 4.1. In the left-hand figures, one of the matchings in $\mathbf{M}(\mathbf{R})$ is depicted using double lines.

Graph $G(\mathbf{R})$ is obtained from T by omitting all edges of $\mathbf{P}$, all end vertices of the edges of $\mathbf{R}$, and all edges incident upon these vertices (Figure 4.1.). Set $\mathbf{G} = \{G(\mathbf{R}) | \mathbf{R} \subseteq \mathbf{P}\}$. Clearly, $m(G(\mathbf{R})) = m(\mathbf{R})$ thus by Eqs. (1) and (2),

$$m(T) = \sum_{\mathbf{R} \subseteq \mathbf{P}} m(\mathbf{R}) = \sum_{r=0}^{p} \sum_{|\mathbf{R}|=r} m(\mathbf{R}) . \quad (3)$$

Direct all edges of $G \in \mathbf{G}$ from top to bottom, thus turning G into a directed (bipartite) graph $\vec{G}$ (Figure 4.2). Every $\vec{G}$ is the embedding of a planar

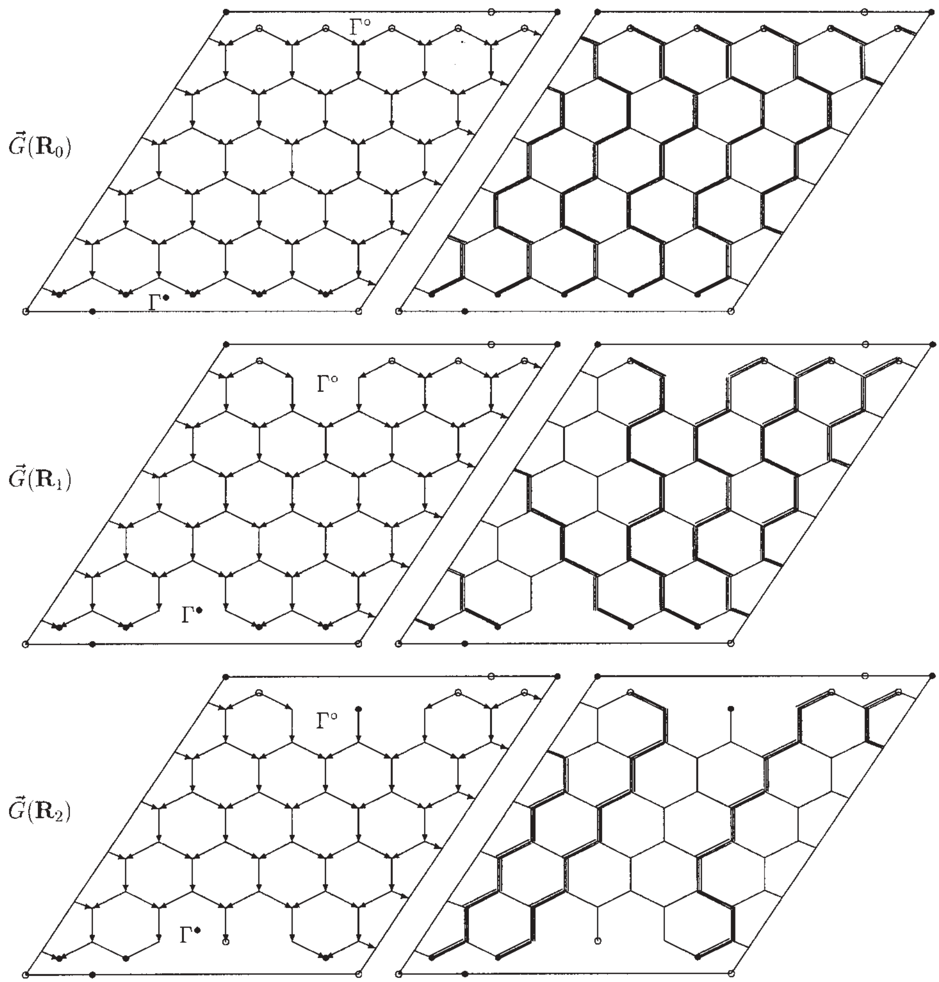


Figure 4.2. Note that the non-vertical edges that belong to $\mathbf{M_i}$ together with the vertical edges that do not belong to $\mathbf{M_i}$ (i = 0, 1, 2) form systems of disjoint monotone paths in $G(\mathbf{R}_i)$ connecting all peaks with all valleys of $G(\mathbf{R}_i)$; these path systems are depicted (see the heavy lines) in the figures on the right-hand side.

(not necessarily connected) directed graph in a cyclinder. Set $\vec{\mathbf{G}} = \{\vec{G} | G \in \mathbf{G}\}$. The white sources (black sinks) of $\vec{G} \in \vec{\mathbf{G}}$ are called its *peaks* (*valleys*). Note that a black source (white sink) is not a peak (valley). As in the case of hexagonal systems in the plane,[3,4] for each $\vec{G} \in \vec{\mathbf{G}}$.

(i) the number of peaks of a graph $\vec{G} = \vec{G}(\mathbf{R})$ is equal to the number of its valleys, namely, $p - r$;

(ii) for each $\mathbf{R} \subseteq \mathbf{P}$ there is a (1,1)-correspondence between the set $\mathbf{M}(\mathbf{R})$ and the set of systems of disjoint monotone paths connecting the peaks of $\vec{G}(\mathbf{R})$ with its valleys such that in every such path system each peak and each valley are the end vertices of exactly one (directed) path (Figure 4.2). Every $\vec{G} \in \vec{\mathbf{G}}$ is the embedding of a planar (not necessarily connected) directed graph in a cylinder.

Some immediate observations.

(a) $\vec{G}(\mathbf{R})$ is the empty graph (without edges and vertices) if and only if $\mathbf{R} = \mathbf{P}$ and $q = 1$. By convention, the number of monotone path systems of the empty graph is assumed to be equal to 1.

(b) If $\vec{G} = \vec{G}(\mathbf{R})$ is non-empty and connected, then it has two particular (in general, non-hexagonal) faces which result from the edge-and-vertex deleting process described above, namely a top face $\Gamma^{\circ} = \Gamma^{\circ}(\vec{G})$ with all sources of $\vec{G}$ on its boundary and a bottom face $\Gamma^{\bullet} = \Gamma^{\bullet}(\vec{G})$ with all sinks of $\vec{G}$ on its boundary (see Figure 4.2.).

(c) If $\vec{G}$ is disconnected with components $\vec{G}_1, \vec{G}_2, \ldots, \vec{G}_c$, then, necessarily, $1 \leq q \leq 2$, and $m(G) = m(G_1) \cdot m(G_2) \cdot \ldots \cdot m(G_c)$. (Note that some component G_γ may have an odd number of vertices, implying $m(G) = 0$.)

KASTELEYN'S ORIENTATION

Graph orientations of the kind to be considered next were first used by P. W. Kasteleyn[5] in his pioneering work on dimer coverings of the square lattice graph. Let $\vec{G}$ be any directed plane graph – *i.e.*, an embedding of a directed planar graph in the plane – with an even number of vertices. Let $\omega = \omega(\vec{G})$ denote the orientation of $\vec{G}$, and let Γ be a (finite or infinite) face of G. Orientation ω is said to be *Kasteleyn with respect to* Γ iff, for each component C of the boundary of Γ, the number of arcs of C whose left bank belongs to Γ is odd; ω is *Kasteleyn* for G iff ω is Kasteleyn with respect to all faces (including the infinite face) of G.

It is not difficult to prove that a (finite) plane graph G has a Kasteleyn orientation if and only if each component of G has an even number of vertices. Thus, if G does not have a Kasteleyn orientation, then $m(G) = 0$. Let G be a plane graph equipped with a Kasteleyn orientation and let $\boldsymbol{A} = (a_{i,j})$ denote its Kasteleyn adjacency matrix defined by

$$a_{ij} = \begin{cases} 1 & \text{if there is an are from vertex } i \text{ to vertex } j, \\ -1 & \text{if there is an arc from vertex } j \text{ to vertex } i, \\ 0 & \text{otherwise.} \end{cases}$$

Kasteleyn's Theorem.[5,6]

$$m(G) = \sqrt{det\, \mathbf{A}}\ . \tag{4}$$

For $\mathbf{R} \subseteq \mathbf{P}$, besides $\omega_1 = \omega(\vec{G}(\mathbf{R}))$, consider the orientation ω_2 that is obtained from ω_1 by reversing the direction of all arcs intersected by the line segment $\gamma = AB_1'''$ of P (Figures 2, 3). Clearly, both orientations ω_1, ω_2 are Kasteleyn with respect to every hexagon of every graph $G(\mathbf{R})$, $\mathbf{R} \subseteq \mathbf{P}$; in addition, it is easy to check that ω_ρ is Kasteleyn with respect to both Γ° and $\Gamma^\bullet$ if and only if $p - r \equiv \rho$, *mod* 2. Define $\lambda = \lambda(\mathbf{R})$ by $\lambda \in \{1,2\}$, $\lambda \equiv p - r$, *mod* 2. The above now yields

Lemma 1.
Orientation $\omega_{\lambda(\mathbf{R})}$ is Kasteleyn for $G(\mathbf{R})$. □

For $\lambda = 1, 2$ and for every directed edge (arc) $a \in E(\vec{G})$ define $\sigma_\lambda(a)$ by

$$\sigma_1(a) = 1,\ \sigma_2(a) = \begin{cases} -1 & \text{if } a \text{ is intersected by } \gamma \\ 1 & \text{otherwise} \end{cases}$$

CALCULATING THE NUMBER OF KEKULÉ STRUCTURES

For $T \in \mathbf{T}$ we shall now determine the numbers $m(\mathbf{R})$ and $m(T)$ (see equation (3)).

We start with $\mathbf{R} = \emptyset$ and set $\vec{G}(\emptyset) = \vec{G}_0$.

Let $\{x_1, x_2,..., x_p\}$ and $\{y_{1-t}, y_{2-t},..., y_{p-t}\}$ (labelled from left to right), be the set of peaks and the set of valleys of $\vec{G}_0$, respectively. Recall that t stands for the torsion, the subscripts $1 - t$, $2 - t$,..., $p - t$ are to be reduced to the smallest positive residues modulo p.

Algorithm A (see Figure 5):

The entries are arranged as indicated in Figure 5a. For $\lambda = 1, 2$ assign to every vertex z of $\vec{G}_0$ a vector $\boldsymbol{w}_\lambda(z) = (w_{\lambda 1}(z), w_{\lambda 2}(z),..., w_{\lambda \mathrm{p}}(z))$ according to the following rules.

(A.1) Start with the sources.
For peak x_i $(i = 1, 2,..., p)$, set $\boldsymbol{w}_\lambda(x_i) = (\delta_{i1}, \delta_{i2},..., \delta_{ip})$ where $\delta_{ii} = 1$ and $\delta_{ij} = 0$ iff $i \neq j$.
For a black source y, set $\boldsymbol{w}_\lambda(y) = (0, 0,..., 0)$ $(\lambda = 1, 2)$.

(A.2) For every vertex z of $\vec{G}_0$ that is not a source, following the arrows of $\vec{G}_0$ calculate the vectors

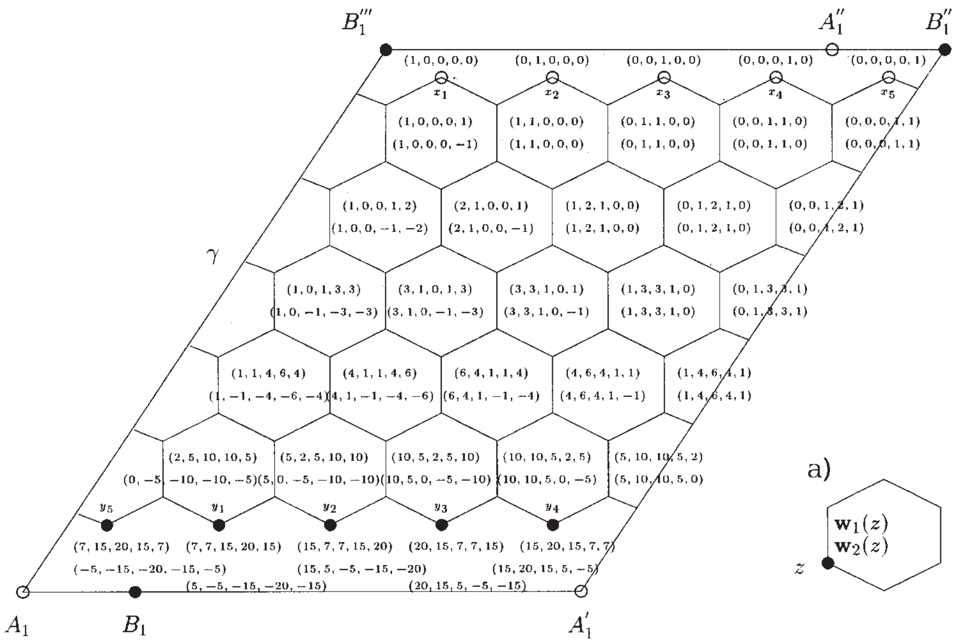


Figure 5. The entries are arranged as indicated in Figure 5a.

$$\boldsymbol{w}_\lambda(z) = \sum \sigma_\lambda(z', z) \cdot \boldsymbol{W}_\lambda(z'), \ (\lambda = 1, 2),$$

where the sum is taken over the one or two predecessors z' of z.

(A.3) For valley y_j, $j = 1, 2,\ldots, p$, let $w_{\lambda,ij} = w_{\lambda i}(y_j)$ and $\boldsymbol{w}_\lambda(y_j) = (w_{\lambda 1j}, w_{\lambda 2j},\ldots, w_{\lambda,pj})$.
Form the $p \times p$-matrices

$$\begin{aligned}\boldsymbol{W}_\lambda(t) &= \boldsymbol{W}_\lambda(\vec{G}_0)\\ &= (\boldsymbol{w}_\lambda^{\mathrm{T}}(y_1), \boldsymbol{w}_\lambda^{\mathrm{T}}(y_2),\ldots, \boldsymbol{w}_\lambda^{\mathrm{T}}(y_p))^{\mathrm{T}}\\ &= (w_{\lambda,ij}),\end{aligned}$$

$i, j = 1, 2,\ldots p$ $(\lambda = 1, 2)$.

It is not difficult to see that the matrices $\boldsymbol{W}_1(0)$, $\boldsymbol{W}_2(0)$ resulting from the above algorithm can also be written as powers of the circulant $Z_+ = circ\ (1, 0,\ldots, 0, 1)$ and the skew circulant $Z_- = scirc(1, 0,\ldots, 0, -1)$, respectively, namely, $\boldsymbol{W}_1(0) = Z^q{}_+$, $\boldsymbol{W}_2(0) = Z^q{}_-$ (see Ref. 7). From $\boldsymbol{W}_\lambda(0)$ matrix $\boldsymbol{W}_\lambda(t)$ is obtained just by rotating (*i.e.*, cyclically permuting) the rows of $\boldsymbol{W}_\lambda(0)$: the $(t + 1)st$ row of $\boldsymbol{W}_\lambda(0)$ multiplied by $(-1)^{\lambda-1}$ becomes the first row of $\boldsymbol{W}_\lambda(t)$, *etc.*

(A.4) For $\mathbf{R} \subseteq \mathbf{P}$, set $r = |\mathbf{R}|$ $(0 \le r \le p)$. Clearly, the graph $G(\mathbf{R})$ is an induced subgraph of $G(\emptyset)$ with precisely $p - r$ peaks and as many valleys. Let $\boldsymbol{W} = \boldsymbol{W}(\mathbf{R})$ denote the principal submatrix of $\boldsymbol{W}_{\lambda(\mathbf{R})} = \boldsymbol{W}_{\lambda(\mathbf{R})}(t)$ that corresponds to the complement of $\mathbf{R}$. Note that $\boldsymbol{W}(\mathbf{R})$ is a square matrix of order $p - r$, obtained from $\boldsymbol{W}_{\lambda(\mathbf{R})}$ by deleting all those rows and columns that correspond to the elements of $\mathbf{R}$. By Kasteleyn's theorem (formula (4), specified for bipartite graphs),

Lemma 2.

$$m(\mathbf{R}) = |det\ \boldsymbol{W}(\mathbf{R})| . \qquad \square \quad (5)$$

The extreme cases

1. $\mathbf{R} = \mathbf{P}$, $p - r = 0$.

   $G(\mathbf{P})$ has no peak and no valley, $\boldsymbol{W}(\mathbf{P})$ is the empty matrix. $G(\mathbf{P})$ has exactly one perfect matching which consists of all vertical edges (all edges perpendicular to s). Thus, in accordance with Eq. (5),

   $m(\mathbf{P}) = |det\ \mathbf{W}(\mathbf{P})| = 1$.

2. $\mathbf{R} = \emptyset$, $p - r = p$.

   In this simple case, we do not need Lemma 2: by immediate inspection we see that none of the vertical edges can belong to a perfect matching of $G(\emptyset)$ implying

$$m(\emptyset) = s^q.$$

Equations (3) and (5) now allow $m = m(T)$ to be calculated:

$$m(T) = \sum_{\mathbf{R} \subseteq \mathbf{P}} m(\mathbf{R}) = \sum_{\mathbf{R} \subseteq \mathbf{P}} |det\ \boldsymbol{W}(\mathbf{R})| . \qquad (6)$$

Let $\mathbf{P} = \{1, 2, ..., p\}$ be the set of edges intersected by s where edge i is incident upon peak v_i (see Figures 3).

Call two sets $\mathbf{R}, \mathbf{R}' \subseteq \mathbf{P}$ *cyclically equivalent* (briefly: *c-equivalent*) iff $\mathbf{R}'$ is obtained from $\mathbf{R}$ by shifting the subscripts defining $\mathbf{R}$ modulo p. Clearly, for all members $\mathbf{R}$ of a c-equivalence class the graphs $G(\mathbf{R})$ are isomorphic, thus it suffices to calculate $m(\mathbf{R}) = |det\ \boldsymbol{W}(\mathbf{R})|$ for only one representative $\mathbf{R}$ of each c-equivalence class C and multiply by $\mu = \mu(\mathbf{R}) = |C|$.

Note that the above algorithm is applicable for any (not necessarily canonic) representation (p_i, q_i, t_i) $(i = 1, 2, 3)$ of T.

For our example, the calculations and results are summarized in Table I, which is self-explanatory.

To make the situation more transparent, *m(T)* is calculated a second time in Table II, where another (non-canonical) representation of T-namely with $p_2 = 6$, $q_2 = 5$, $t_2 = 0$ (see Table II) – is used.

TABLE I

(see Figure 3)

R	r	μ	λ	**W**	m	$\mu \cdot m$
Ø	0	1	1	$\boldsymbol{W}_1$	$2^6 = 64$	64
$\{1\}$	1	5	2	$\begin{pmatrix} 5 & -5 & -15 & -20 \\ 15 & 5 & -5 & -15 \\ 20 & 15 & 5 & -5 \\ -15 & -20 & -15 & -5 \end{pmatrix}$	3125	15625
$\{1,2\}$	2	5	1	$\begin{pmatrix} 7 & 7 & 15 \\ 15 & 7 & 7 \\ 20 & 15 & 7 \end{pmatrix}$	1128	5640
$\{1,3\}$		5	1	$\begin{pmatrix} 7 & 15 & 20 \\ 20 & 7 & 7 \\ 15 & 15 & 7 \end{pmatrix}$	2983	14915
$\{1,2,3\}$	3	5	2	$\begin{pmatrix} 5 & -5 \\ -15 & -5 \end{pmatrix}$	100	500
$\{1,2,4\}$		5	2	$\begin{pmatrix} 5 & -15 \\ 20 & -5 \end{pmatrix}$	325	1625
$\{1,2,3,4\}$	4	5	1	(7)	7	35
$\{1,2,3,4,5\}$	5	1	2	Ø	1	1
$\sum$		$2^5 = 32$	/	/	/	$m(T) = 38405$

TABLE II

R	r	μ	λ	**W**	m	$\mu \cdot m$
Ø	0	1	2	$\boldsymbol{W}_2$	$2^5 = 32$	32
$\{1\}$	1	6	1	$\begin{pmatrix} 1 & 1 & 5 & 10 & 10 \\ 5 & 1 & 1 & 5 & 10 \\ 10 & 5 & 1 & 1 & 5 \\ 10 & 10 & 5 & 1 & 1 \\ 5 & 10 & 10 & 5 & 1 \end{pmatrix}$	1296	7776
$\{1,2\}$	2	6	2	$\begin{pmatrix} 1 & -1 & -5 & -10 \\ 5 & 1 & -1 & -5 \\ 10 & 5 & 1 & -1 \\ 10 & 10 & 5 & 1 \end{pmatrix}$	621	3726

R	r	μ	λ	$\boldsymbol{W}$	m	$\mu \cdot m$
Ø	0	1	2	$\boldsymbol{W}_2$	$2^5 = 32$	32
$\{1,3\}$		6	2	$\begin{pmatrix} 1 & -5 & -10 & -10 \\ 10 & 1 & -1 & -5 \\ 10 & 5 & 1 & -1 \\ 5 & 10 & 5 & 1 \end{pmatrix}$	1896	11376
$\{1,4\}$		3	2	$\begin{pmatrix} 1 & -1 & -10 & -10 \\ 5 & 1 & -5 & -10 \\ 10 & 10 & 1 & -1 \\ 5 & 10 & -5 & 1 \end{pmatrix}$	2561	7683
$\{1,2,3\}$	3	6	1	$\begin{pmatrix} 1 & 1 & 5 \\ 5 & 1 & 1 \\ 10 & 5 & 1 \end{pmatrix}$	76	456
$\{1,2,4\}$		6	1	$\begin{pmatrix} 1 & 5 & 10 \\ 10 & 1 & 1 \\ 10 & 5 & 1 \end{pmatrix}$	396	2376
$\{1,2,5\}$		6	1	$\begin{pmatrix} 1 & 1 & 10 \\ 5 & 1 & 5 \\ 10 & 10 & 1 \end{pmatrix}$	396	2376
$\{1,2,5\}$		2	1	$\begin{pmatrix} 1 & 5 & 10 \\ 10 & 1 & 5 \\ 5 & 10 & 1 \end{pmatrix}$	976	1952
$\{1,2,3,4\}$	4	6		$\begin{pmatrix} 1 & -1 \\ 5 & 1 \end{pmatrix}$	6	36
$\{1,2,3,5\}$		6	22	$\begin{pmatrix} 1 & -5 \\ 10 & 1 \end{pmatrix}$	51	306
$\{1,2,4,5\}$		3	2	$\begin{pmatrix} 1 & -10 \\ 10 & 1 \end{pmatrix}$	101	303
$\{1,2,3,4,5\}$	5	6	1	(1)	1	6
$\{1,2,3,4,5,6\}$	6	1	2	Ø	1	1
$\sum$		$2^6 = 64$	/	/	/	$m(T) = 38405$

For $T = (p, q, t)$ write $m(T) = m\ (p, q, t)$.

In order to show that $m(T)$ depends on the torsion t of T, we calculated $m(5, 6, t)$ for $t = 0, 1, 2, 3, 4$ and obtained

$$m(5, 6, 0) = m(5, 6, 1) = 38405,$$
$$m(5, 6, 2) = m(5, 6, 4) = 38405,$$
$$m(5, 6, 3) = 39440 \text{ (see also Ref. 8).}$$

REFERENCES

1. a) Jie Liu, Hongjie Dai, J. H. Hafner, D. T. Colbert, R. E. Smalley, S. J. Tans, and C. Dekker, *Nature* **385** (1997) 780–781;
   b) M. Randić, Y. Tsukano, and H. Hosoya, *Kekule' Structures for Benzenoid Tori*, Natural Science Report, Ochanomizu University, Vol. 45, No. 2, 1994, 101–119.
2. E. C. Kirby, R. B. Mallion, and P. Pollak, *J. Chem. Soc. Faraday Trans*. **89** (1993) 1945–1953.
3. P. John and H. Sachs, *Calculating the Number of Perfect Matchings and of Spanning Trees, Paulings Orders, the Characteristic Polynomial, and the Eigenvectors of a Benzenoid System,* in: *Advances in the Theory of Benzenoid Hydrocarbons* (Ed. I. Gutman and S. J. Cyvin), *Topics in Current Chemistry* **153** (1990) 145–179.
4. P. John and H. Sachs, *J. Chem. Soc. Faraday Trans.* **86** (1990) 1033–1039.
5. P. W. Kasteleyn: *Graph Theory and Crystal Physics*, in: *Graph Theory and Theoretical Physics,* F. Harary (Ed.), Academic Press London, 1967, pp. 43–110.
6. H. Sachs, P. Hansen, and M. Zheng: *Kekulé Count in Tubular Hydrocarbons*, *MATCH-Communications in Mathematical an in Computer Chemistry*, **33** (1996) 169–241.
7. P. J. Davis: *Circulant Matrices*, John Wiley & Sons, New York, Chichester, Brisbane, Toronto, 1979.
8. P. E. John and B. Walther: *Sketch About Possible Structures and Numbers of Perfect Matchings of Toroidal Hexagonal Systems*, preprint N^{o}. M 08/94 (TU Ilmenau).

SAŽETAK

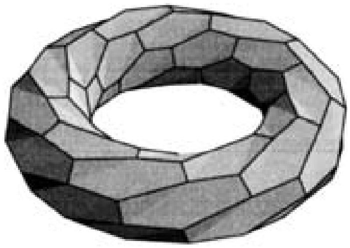
Broj Kekuléovih struktura u torusnim heksagonalnim ugljikovim kavezima

Peter E. John

Nakon otkrića fullerena, prirodno se postavilo pitanje postojanja čisto ugljikovih heksagonalnih kaveza u obliku torusa koje bismo mogli nazvati »torusnim grafitom«. Istaknimo da je torus jedina zatvorena površina S na koju su mogu smjestiti trovalentni grafovi G čija su sva lica heksagoni (Ref. 1a, Slika 1). Predloženo je da se takove molekule i pripadni im molekularni grafovi zovu *torenima*.

Napomenimo da su se ovom temom prvi puta bavili M. Randić, Y. Tsukano i H. Hosoya.[1b]

Ovdje je prikazan algoritam koji omogućava izračunavanje broja Kekuléovih struktura torena u polinomskom vremenu.



Slika 1