An Algorithm for Counting Spanning Trees in Labeled Molecular Graphs Homeomorphic to Cata-Condensed Systems

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The algorithmic method of Gutman and Mallion (1993), for calculating the number of spanning trees in the (labeled) molecular graphs of cata-condensed systems containing rings of only one size, was subsequently generalized by John and Mallion (1996) to make it applicable to such systems comprising rings of more than one size; this latter algorithm is thus generally valid for enumerating the spanning trees in the molecular graphs of any cata-condensed system. This algorithmic philosophy is extended here in order to devise a procedure that is suitable for an even more general class of molecular graphs—namely, those *homeomorphic to* the molecular graphs of cata-condensed systems. An example of its use is illustrated by explicitly computing the numerical value for the complexity of a (hypothetical) pentacyclic network consisting of two four-membered rings, two five-membered rings, and a nine-membered ring, giving rise to a spanning-tree count entirely in accord with that predicted *via* the theorem of Gutman, Mallion, and Essam (1983)—on the face of it, an apparently very different approach, based on the "generalized characteristic polynomial" of the inner dual of the graph in question.

1. INTRODUCTION

In recent years, we and others[1−14] have extensively considered the counting of spanning trees in labeled molecular graphs, with particular emphasis on the novel family of carbon clusters now known as the fullerenes.[2,5,7,9,10,12−14] The initial motivation for this was the relevance of spanning trees[15−17] in calculating the magnetic properties of conjugated systems *via* the "ring-current" model[18,19] in the context of classical π-electron molecular orbital theory.[20,21] In a previous work,[6] two of the present authors devised a method that was suitable for calculating the *complexities* of (*i.e.*, the number of spanning trees in) the labeled molecular graphs of cata-condensed systems containing rings of only one size. In a later publication,[11] another combination of two of us generalized this to such systems containing rings of more than one size. The algorithm presented in ref 11 is generally applicable to cata-condensed cell systems—*i.e.*, those in which two finite adjacent cells (see section 2) have exactly one edge in common and all vertices lie on the boundary of the infinite region (see, for example, the graph shown in Figure 1.1). In the present communication, we offer a new algorithm, one that is applicable to a more general class of graphs—namely to graphs homeomorphic to *cata-condensed cell systems*; the graph in Figure 1.2 is an example of such. The latter is sometimes also called a *subdivision,* defined as follows *(e.g.*, ref 22): graph G′ is a subdivision of graph *G* if *G*′ can be obtained from *G* by replacing edges by paths (of length ≥ 1). It should be noted that in adding vertices of degree two to graphs—as in going from *O* (Figure 1.1) to *S* (Figure 1.2)—an operation is performed that is the reverse of the one proposed by Balaban *et al.*[23] in the process of counting rings in graphs.

2. DEFINITIONS AND NOTATION (SEE FIGURE 1)

Let *Z* be a positive integer greater than 1. A *cell* is a closed plane region bounded by a *Z*-gon with side of unit length. A *cell system* is a finite 2-connected planar graph[4] in which every finite region is a cell. A *spindle graph* is a finite connected planar graph whose finite regions are 2-cells (see Figure 1.4). The *inner dual, D*(*G*), of a finite 2-connected planar graph *G* is the dual of *G* without the vertex that corresponds to the infinite region of *G* and without all the edges that are incident upon that vertex[1] (see Figures 1.3 and 1.4). A *spindle cell system* is a cell system whose inner dual is a spindle graph (see Figure 1.2). The set of all spindle cell systems is denoted by *S*. A *cata-condensed cell system* is a cell system whose inner dual is a tree[4] (see Figure 1.1). (Note that a cata-condensed cell system is a spindle cell system, but the reverse is not necessarily true. Note also that our terminology differs somewhat from that originally introduced by Balaban and Harary.[24]) A *matching* of a graph *G* is a set of pairwise disjoint edges. A *spanning tree* of a graph G is a tree that covers all the vertices of

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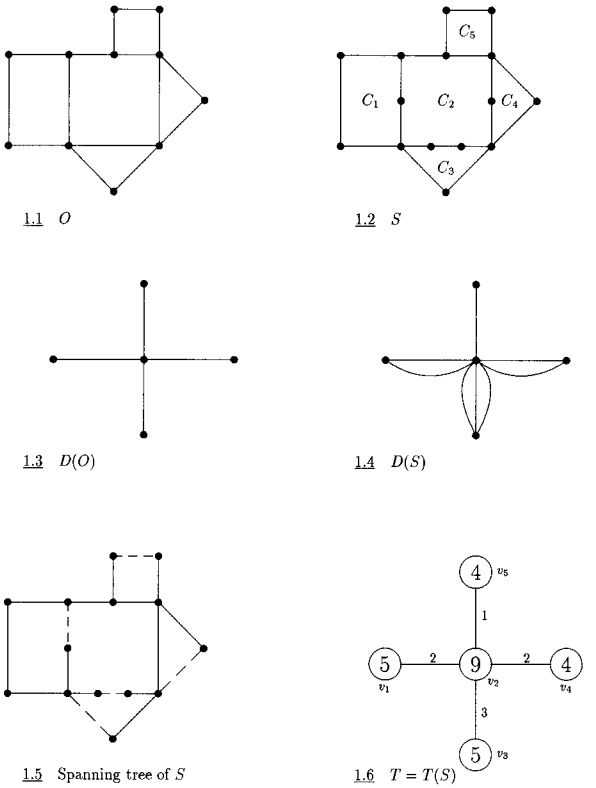

Figure 1. Some representations of spindle cell systems: 1.1, a cata-condensed cell system *O*; 1.2, a spindle cell system *S*; 1.3, inner dual of graph *O*; 1.4, inner dual of graph *S*; 1.5, a spanning tree of *S*; 1.6, a tree representation, *T* (*S*), of *S*.

G[1,15]; (see Figure 1.5). The number of spanning trees of $S \in \mathsf{S}$ is denoted by $t = t(S)$.

Observation 1: Every spindle cell system has a spanning tree.

3. SPANNING TREES IN A SPINDLE CELL SYSTEM

3.1. The Matrix Tree Theorem.[15−17] Let $S \in \mathsf{S}$ be a spindle cell system with $n = n(S)$ vertices, $m = m(S)$ edges and for $c = c(S) = m - n + 1$, denote by $\mathsf{C} = \mathsf{C}(S) = \{C_1, C_2, ..., C_c\}$ the set of cells of *S*.

Observation 2: If $c = c(S) = 1$, then $t(S) = m = n$.

Suppose that *S* has more than one cell. For $i, j = 1, 2, ...,$ c and $C_i, C_j \in \mathsf{C}$, define numbers b_{ij} such that, for $i \neq j$, b_{ij} is minus the number of common edges of the cells C_i, C_j (with the possibility that $b_{ij} = 0$), whereas for $i = j$, b_{ij} is the number of edges (or vertices) of the cell C_i. The quantities b_{ij} may be considered to constitute the elements of a square matrix $\mathbf{B} = \mathbf{B}(S) = (b_{ij})$.

Theorem:[1]

$$t(S) = \det \mathbf{B}(S) \tag{1}$$

Clearly, in the present case, matrix **B** represents an edge- and vertex-weighted tree $T = T(S)$ with vertex set $V(T) = \{v_1, v_2, ..., v_c\}$ and edge set $E(T)$. Vertex $v_i \in V(T)$, which corresponds to cell C_i of *S*, has weight $w(v_i) = b_{ii}$. When $i \neq j$ and $b_{ij} \neq 0$, then the edge $e = (v_i, v_j)$ is encountered. The weight, $w(e)$, of this edge is chosen to be $-b_{ij}$, and all weights of *T* are then positive (Figure 1.6). The determinant appearing in eq 1 may thus be written as

$$\tau(T) = \det \mathbf{B}(S) \tag{2}$$

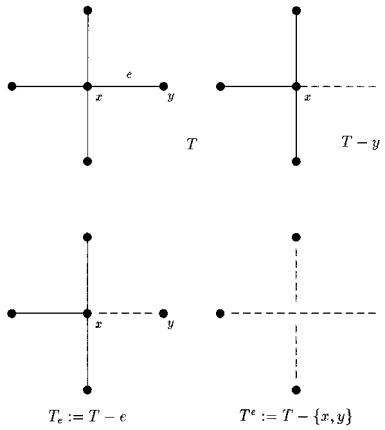

Figure 2. Reduction figures for a tree, *T*.

3.2. A Recursion Formula for $\tau(T)$. Let $T = T(S)$ for a given $S \in \mathsf{S}$ and let $M = M(T)$ and $M_k = M_k(T)$ denote the set of all matchings and the set of all matchings with exactly $k = 0, 1, 2, ...[c/2]$ edges of *T*, respectively. (Recall that, for a real number *x*, the symbol $[x]$ denotes the largest integer that is not greater than *x*.) It is clear that graph $H \in M_k$ has exactly $2k$ vertices. A well-known formula for calculation of $\tau(T)$ is quoted by Cvetković, Doob, and Sachs.[15] It is as follows:

$$\tau(T) = \sum_{H \in M(T)} \{(-1)^{p(H)} w(H)\} \tag{3.1}$$

or

$$\tau(T) = \sum_{k=0}^{[c/2]} \{(-1)^k \sum_{H \in M_k(T)} w(H)\} \tag{3.2}$$

where

$$w(H) = \prod_{e \in E(H)} \{w(e)\}^2 \cdot \prod_{v \in V(T) - V(H)} w(v) \tag{4}$$

and $p(H)$ stands for the number of components—in this case, the number of edges—of *H*. Note that, by definition, $w(\varnothing) := 1$. Equation 3.2 gives an indication of how $\tau(T)$ may be calculated by a recursive procedure. Let $e = (x,y)$ be an edge of *T*. Then put $T_e := T - e$, and $T^e := T - x - y$ (*i.e.*, $T^e := T - \{x,y\}$). (See Figure 2.)

Define the following matching sets of *T* (with respect to *e*):

$$M_e := M(T_e)$$

$$\bar{M}_e := M(T) - M(T_e)$$

and

$$M^e := M(T^e)$$

Clearly, $\bar{M}_e$ is the set of matchings of *T* that contain edge $= (x,y)$, and M_e *is* the set of such matchings that do not contain edge *e*. From eqs 3, we can deduce that

$$\tau(T) = \sum_{H \in M_e(T)} (-1)^{p(H)} w(H) + \sum_{\bar{H} \in \bar{M}_e(T)} (-1)^{p(\bar{H})} w(\bar{H}) \tag{5}$$

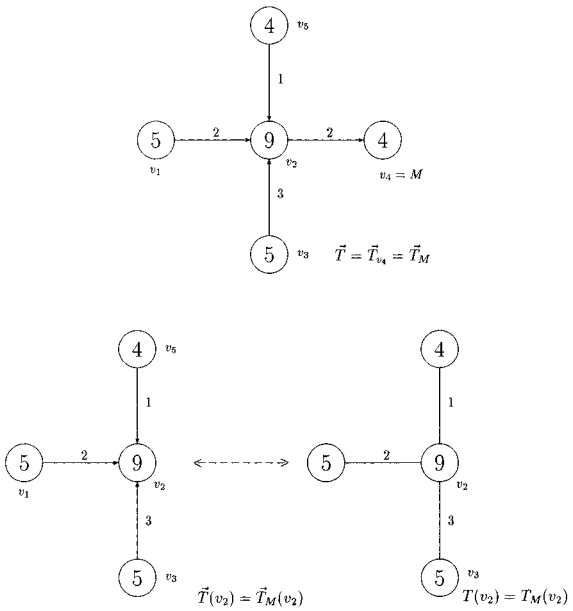

Figure 3. River T and subriver $T(v_2)$ (which corresponds to a subtree $T(v_2)$ of T with respect to M).

Note that for $\bar{H} \in \bar{M}_e$ it is true that $\bar{H} - \{x, y\} \in M^e$. Therefore

$$\sum_{\bar{H} \in \bar{M}_e(T)} (-1)^{p(\bar{H})} w(\bar{H}) = -\{w(e)\}^2 \cdot \sum_{H' \in M^e(T)} (-1)^{p(H')} w(H') \quad (6)$$

Inserting eq 6 into eq 5, and bearing in mind eq 3.1, gives

$$\tau(T) = \sum_{H \in M(T_e)} (-1)^{p(H)} w(H) - \{w(e)\}^2 \cdot \sum_{H' \in M(T^e)} (-1)^{p(H')} w(H') = \tau(T_e) - \{w(e)\}^2 \cdot \tau(T^e) \quad (7)$$

This is the fundamental equation of our recursive procedure.

3.3. The Algorithm. Preparatory Remarks. (a) Let $S = C$ be an isolated cell; then $t(S) = t(C) = n(C)$.

(b) Let $S \in \mathcal{S}$ with at least two cells and let $T = T(S)$ be the (edge- and vertex-) weighted tree, as described above. Select a vertex M of T and direct all edges toward it. Thus, in a figurative and intuitive sense, T may be regarded as being turned into a "river", $\vec{T} = \vec{T}_M$, with its tributaries, its sources, and its mouth, M—*cf.* refs 7 and 11—the latter also called by Gordon[25] an "estuary". (Note that a source vertex is a vertex other than the mouth vertex whose degree is one.) The end cells corresponding to the sources are thus called the source cells, and the end cell corresponding to the mouth is called the mouth cell.[7,11] *Every* vertex v (different from M) of $\vec{T}_M$ is a mouth vertex of a "subriver", $\vec{T}(v) = \vec{T}_M(v)$, with respect to mouth M, of T. Note that subriver $\vec{T}(v)$ is a river, $\vec{T}_v$, of a subtree of T which we denote by $T(v) = T_M(v)$. (See Figure 3.) Note also that, trivially, if v is a source of $\vec{T}$, then subriver $T(v)$ and the corresponding subtree

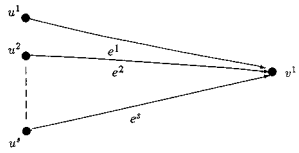

Figure 4. Reduction figure.

are identical graphs with one vertex v and no edge. Starting from the sources, and following the river, we shall reconstruct $\vec{T}$ from its vertices in a stepwise fashion and shall, in the process, simultaneously calculate the numbers $r(v) := \tau(T(v))$, and $h(v) := \tau(\underline{T}(v) - v)$ for every vertex v and for the mouth vertex M of $\vec{T}$. Then, in particular,

$$r(M) = \tau(T) = t(S) \quad (8)$$

Let $(\vec{u,v})$ denote a directed edge of $\vec{T}$ that starts at vertex u and ends at vertex v. For vertex v of $\vec{T}$ we define the set

$$N(v) := \{(u,v), u \in V(T)\}$$

Algorithm. As in our previous work,[7] when, in the course of this algorithmic process, we refer to "marking" a given vertex, this should be taken to mean that the quantities indicating such a marking are (at least *notionally*, if not, in practice, actually *physically) written down beside the vertex in question.*

To every vertex v of $\vec{T}$ we assign a vector $(r(v), h(v))$ by means of the following recursive procedure.

(1) Let v^0 be a source vertex of $\vec{T}$ which corresponds to cell C^0 of S. Then *mark* v^0 by the quantity

$$(r(v^0), h(v^0)) := (\tau(v^0), \tau(\varnothing)) = (n(C^0), 1) \quad (9)$$

(2) There exists a vertex v^1 of $\vec{T}$, as yet unmarked, that corresponds to cell C^1 of S, and all vertices of $N(v^1) = \{u^1, u^2, ..., u^s: s \geq 1\}$ are marked by $(r(u^i), h(u^i))$ for $i = 1, 2, ..., s$. Directed edges $e^i = (u^i, v^1)$ have weight $w(e^i)$ and $w(v^1) = n(C^1)$. Write by the side of v^1 the quantity:

$$(r(v^1), h(v^1)) = \left(h(v^1) \cdot \left[w(v^1) - \sum_{i=1}^{s} \{w(e^i)\}^2 \frac{h(u^i)}{r(u^i)}\right], \prod_{i=1}^{s} r(u^i)\right) \quad (10)$$

Proof of eq 10. (See Figure 4.) For $i = 2, 3, ..., s$ define

$$T_{1,2,...,i} := T - e^1 - e^2 - ... - e^i \quad (11)$$

and

$$T^i{}_{1,2,...,i-1} := T - e^1 - e^2 - ... - e^{i-1} - \{u^i, v^1\} = T - \{u^i, v^1\} =: T^i \quad (12)$$

We now successively apply eq 7 for $e = e^1, e^2, ..., e^s$ of T:

$$r(v^1) = \tau(T(v^1)) = \tau(T_1) - \{w(e^1)\}^2 \cdot \tau(T^1)$$

$$= \tau(T_{1,2}) - \{w(e^2)\}^2 \cdot \tau(T_1^2)$$

$$- \{w(e^1)\}^2 \cdot \tau(T^1)$$

$$= ...$$

$$= \tau(T_{1,2,...,s}) - \{w(e^s)\}^2 \cdot \tau(T^s_{1,2,...,s-1})$$

$$- \{w(e^{s-1})\}^2 \cdot \tau(T^{s-1}_{1,2,...s-1}) - ...$$

$$- ... - \{w(e^1)\}^2 \cdot \tau(T^1)$$

Taken in conjunction with eqs 12, these give

$$r(v^1) = \tau(T_{1,2,...,s}) - \sum_{i=1}^{s} \{w(e^i)\}^2 \cdot \tau(T^i)$$

$$= w(v^1) \cdot \prod_{i=1}^{s} r(u^i) - \sum_{i=1}^{s} \{w(e^i)\}^2 \cdot h(u^i) \cdot \prod_{i \neq j=1}^{s} r(u^j)$$

$$= \prod_{i=1}^{s} r(u^i) \cdot \left[w(v^1) - \sum_{i=1}^{s} \{w(e^i)\}^2 \frac{h(u^i)}{r(u^i)} \right]$$

And

$$h(v^1) = \tau(T(v^1) - v^1)$$

$$= \prod_{i=1}^{s} r(u^i)$$

Note that for $s = 1$,

$$r(v^1) = w(v^1) \cdot r(u^1) - \{w(e^1)\}^2 \cdot h(u^1)$$

and

$$h(v^1) = r(u^1)$$

4. EXAMPLE OF THE ALGORITHM

We give here a specific example of application of the algorithm, to the graph shown in Figure 1. In the first treatment, illustrated in Figure 5.1, we select the mouth-vertex, M, to be v_4—*i.e.*, we set $\vec{T} = \vec{T}_{v_4}$. Then, by virtue of eq 9, we deduce that

$$(r(v_1), h(v_1)) = (r(v_3), h(v_3)) = (5,1)$$

and

$$(r(v_5), h(v_5)) = (4,1)$$

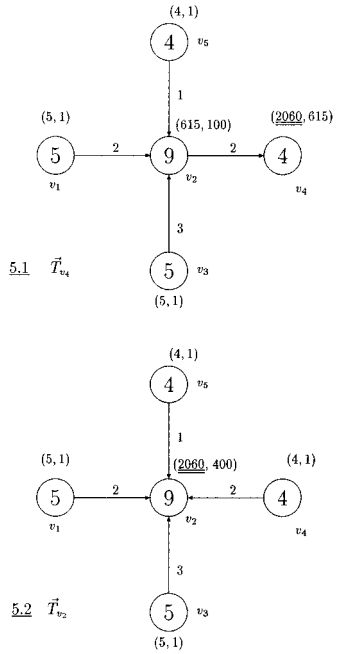

Figure 5. Example of use of the algorithm to calculate the number of spanning trees in the graph shown in Figure 1: 5.1, with the mouth vertex, M, selected to be v_4; and 5.2, with v_2 selected as the mouth vertex, M.

Furthermore, because of eq 10,

$$h(v_2) = 5^2 \cdot 4 = 100$$

and

$$r(v_2) = 100\left[9 - \left(4 \cdot \frac{1}{5} + 9 \cdot \frac{1}{5} + 1 \cdot \frac{1}{4}\right)\right] = 615$$

Finally,

$$h(M = v_4) = r(v_2) = 615$$

and

$$r(M = v_4) = 615\left[4 - 4 \cdot \frac{100}{615}\right] = 2060 = t(S)$$

Hence, the number of spanning trees of the graph in question (Figure 1) is seen to be 2060.

In an alternative, but entirely equivalent, strategy, we could, for example, select the mouth, M, to be the vertex v_2 (*i.e.*, we set $\vec{T} = \vec{T}_{v_2}$)—as depicted in the scheme shown in Figure 5.2. In this case, the following workings would apply

$$(r(v_1), h(v_1)) = (r(v_3), h(v_3)) = (5,1)$$

and

$$(r(v_4), h(v_4)) = (r(v_5), h(v_5)) = (4,1)$$

(both from eq 9), and, by virtue of eq 10, we have, as before, that

$$h(v_2) = 5^2 \cdot 4^2 = 400$$

and so, finally,

$$r(v_2) = 400\left[9 - 4\cdot\frac{1}{5} - 9\cdot\frac{1}{5} - 4\cdot\frac{1}{4} - 1\cdot\frac{1}{4}\right]$$

$$= 400\cdot\frac{103}{20} = 2060 = t(S)$$

thereby confirming, albeit *via* different intermediate numbers, that the complexity of the graph illustrated in Figure 1 is 2060.

5. CONCLUDING REMARKS

Our previous algorithm, recently described,[11] is applicable only to outer-planar graphs—*i.e.*, those in which two finite adjacent cells have exactly one edge in common; (see, for example, Figure 1.1). The new algorithm that we have proposed in the present paper is more general in that it is applicable to graphs homeomorphic to (*i.e.*, that are subdivisions of) a cata-condensed system; (see, for example, Figure 1; *S* is a subdivision of *O*). Our algorithm is appropriate also for *some* peri-condensed cell systems. It is essentially a stepwise and systematized form for the calculation, by means of the method devised in ref 1, of the determinant $\mathbf{B} = \mathbf{B}(S)$. The illustrative example given in the previous section could, indeed, have been dealt with, and its spanning-tree count of 2060 confirmed, *via* an application of the theorem due to two of us and Essam,[1] which would predict the complexity of the (planar) graph in question—Figure 1.1—to be the value of (for example) the determinant

$$\left|\begin{pmatrix} 5 & -2 & 0 & 0 & 0 \\ -2 & 9 & -3 & -2 & -1 \\ 0 & -3 & 5 & 0 & 0 \\ 0 & -2 & 0 & 4 & 0 \\ 0 & -1 & 0 & 0 & 4 \end{pmatrix}\right|$$

which is 2060.

As was emphasized in the context of our earlier algorithm,[10] physical and chemical interest in the spanning trees extant within the *molecular* graphs that represent the connectivity of the atoms in (geometrically) planar, conjugated systems initially arose from a consideration of their magnetic properties.[16−21] If a calculation of the relative π-electron ring-current intensities (and/or their effect on magnetic susceptibilities and ^{1}H-NMR chemical-shifts[20,21,17,18]) were to be carried out on the (hypothetical) conjugated hydrocarbon with carbon-atom connectivity represented by the graph in Figure 1, the unitary transformation[20,21,17,18] encountered in the course of such a ring-current computation may, *au choix*, be based on *any* convenient *one* of the 2060 spanning trees—be it semi-Hamiltonian[20] or non-Hamiltonian[21,17,26]—to be found within the graph that we have been discussing.

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