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A classification of outerplanar K-gonal 2-trees

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Abstract. We give in this work the molecular expansion of the species of outerplanar K-gonal 2-trees, extending previous work on ordinary ($K = 3$) outerplanar 2-trees. This is equivalent to a classification of these graphs according to their symmetries (automorphism groups). We give explicit formulas for all coefficients occuring in this expansion.

Résumé. Dans ce travail, nous donnons la décomposition moléculaire des 2-arbres K-gonaux exterplanaires, prolongeant un travail antérieur sur les 2-arbres habituels (où $K = 3$) exterplanaires. Cela est équivalent à une classification de ces structures selon leurs stabilisateurs. Nous donnons des formules explicites pour tous les coefficients apparaissant dans la décomposition.

1. Introduction

Essentially, a *2-tree* is a simple connected graph composed by triangles glued along their edges in a tree-like fashion, that is, without cycles (of triangles). The enumeration of 2-trees has been extensively studied in the literature. See, for instance, Harary and Palmer [**8**] and Fowler et al [**6**]. Here we consider more general 2-trees, where the triangles are replaced by quadrilaterals, pentagons, or polygons with K sides (K-gons), $K \geq 3$. The term K-*gonal* 2-trees is used when K is fixed, *triangular*, *quadrangular*, *pentagonal*, $\ldots$, for $K = 3, 4, 5, \ldots$, respectively, and *polygonal* 2-trees when the polygon size K is allowed to vary. The labelled, unlabelled and asymptotic enumeration of K-gonal 2-trees for any fixed K is considered in [**12**] and in [**13**], where the perimeter is taken into account. The K-gonal 2-trees are not to be confused with K-dimensional trees, or K-trees, which are built with K-simplices glued together along $(K-1)$-faces in a tree-like fashion. Formulas have been given in [**2**] and [**5**] for the labelled enumeration of K-trees but their unlabelled enumeration is still an open problem.

A graph is called *outerplanar* if it can be embedded in the plane in such a way that every vertex lies on the outer face. Their unlabelled and asymptotic enumeration has been recently carried out by Bodirsky, Fusy, Kang and Vigerske [**3**]. It is easily seen that 2-connected outerplanar graphs can be identified with polygonal 2-trees. Figure 1 shows an example of two pentagonal 2-trees, the first one being outerplanar but not the second one. Notice that the degree of any edge (that is, the number of K-gons incident to it) of an outerplanar K-gonal 2-tree cannot exceed 2. The edge is called *internal* if it is of degree 2 and external otherwise. The enumeration of outerplanar K-gonal 2-trees has been studied by Harary, Palmer and Read [**15, 9**] in connection with the cell growth problem and dissections of a polygon. These structures are also of interest in combinatorial chemistry since for $K = 6$, for example, they correspond to special classes of catacondensed benzenoid hydrocarbons (see Gutman and Cyvin [**7**]). Other values of K, for example, 3, 4, 5, 7 and 8 have also been considered in the chemical literature.

The goal of the present work is to give a more refined classification of unlabelled outerplanar K-gonal 2-trees, according to their symmetries, extending previous work by Labelle et al. [**11**] for ordinary (that is, where $K = 3$) outerplanar 2-trees, in the framework of the combinatorial theory of species of Joyal [**10, 1**]. Our classification is closely related to the symmetry nomenclature used by chemists in the case of plane molecules and is expressed as the *molecular expansion* of the corresponding species.

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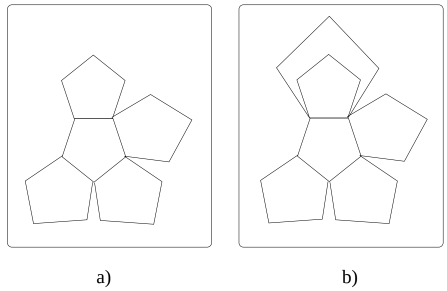


FIGURE 1. Pentagonal 2-trees: a) outerplanar; b) free

We denote by $a = a_K$ the species of outerplanar K-gonal 2-trees, where the underlying set (the labels) is constituted by the K-gons. By convention, the single edge (with an empty set of K-gons) is also considered to be a (*trivial*) 2-tree. The corresponding subspecies is denoted by 1. Another special case is the singleton K-gon whose species is denoted by X. We use the symbols $-$, $\diamond$ and $\underline{\diamond}$ as upper indices to denote the pointing of 2-trees at an edge, at a K-gon and at a K-gon having itself a distinguished edge, respectively. A first step is the extension to the outerplanar K-gonal case of the Dissymmetry Theorem for 2-trees, which links together these various pointed species. The proof, which relies on the concept of *center* of a 2-tree, is similar to the case $K = 3$ and is omitted (see [**6, 11, 12**]).

THEOREM 1.1 (Dissymmetry Theorem). *The species a of outerplanar K-gonal 2-trees satisfies the following isomorphism of species:*

$$a^{-} + a^{\diamond} = a + a^{\underline{\diamond}}. \tag{1.1}$$

□

To achieve our goal, we will compute the molecular expansion of the three auxiliary species a^{-}, $a^{\diamond}$ and $a^{\underline{\diamond}}$, and then use (1.1) to deduce the classification of the species a according to symmetries. There is yet another class of rooted a-structures to introduce. It is the species $A = a^{\rightarrow}$ of outerplanar K-gonal 2-trees where an external edge is selected and oriented. In particular, the rooted edge cannot have more than one K-gon attached to it. An example of such an A-structure is shown in Figure 2 a), for $K = 5$. Except for the trivial one-edge 2-tree, the orientation of the root-edge induces a canonical orientation on all the other edges of its incident K-gon. There are many ways to define this canonical orientation. We use here a convergent orientation as introduced in [**12**] and illustrated in Figure 2, b) and c).

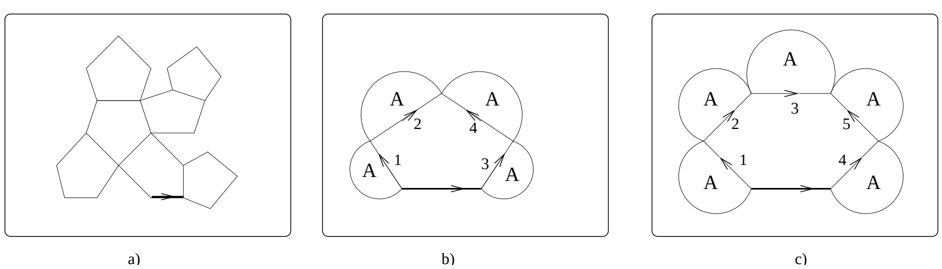


FIGURE 2. a) An A-structure with $K = 5$; b) and c) Induced orientation for K odd and K even, resp.

THEOREM 1.2. *The species A of oriented external edge rooted outerplanar K-gonal 2-trees is characterized by the functional equation*

$$A = 1 + XA^{K-1}. \tag{1.2}$$

PROOF. Any A-structure is either trivial or its root-edge is incident to one K-gon (the factor X in (1.2)) whose other $K-1$ edges inherit a canonical orientation and become the root-edges of new A-structures. See Figure 2, b) and c). These $K - 1$ A-structures can be linearly ordered in a natural way so that we have obtained, in fact, an A^{K-1}-structure. ■

Since oriented-external-edge rooted $\mathfrak{a}$-structures can not have non-trivial symmetries, the species A is asymmetric and admits an expansion of the form

$$A = \sum_{n\geq 0} a_n X^n. \tag{1.3}$$

The coefficients a_n are uniquely determined by (1.2). Lagrange inversion formula can be used to give an expression for a_n and more generally, for the coefficient of X^n in the j^{th} power A^j of A, for $j \geq 0$.

PROPOSITION 1.1. *The coefficient* $a_n^{(j)} := [X^n]A^j(X)$ *is given by* $a_n^{(0)} = \delta_{n0}$ *and, for* $j \geq 1$, $a_0^{(j)} = 1$ *and*

$$a_n^{(j)} = \frac{j}{n}\binom{n(K-1)+j-1}{n-1}, \quad n \geq 1, \tag{1.4}$$

where δ_{ij} *is the Kronecker symbol. In particular, the species* A *admits the expansion*

$$A(X) = 1 + \sum_{n\geq 1} \frac{1}{n}\binom{n(K-1)}{n-1} X^n. \tag{1.5}$$

□

Observe that, when $K = 3$, the numbers $a_n = a_n^{(1)}$ are the famous Catalan numbers. For $K \geq 4$, these numbers are often called *generalized Catalan number*. See sequences A001764, for $K = 4$, A002293 for $K = 5$, A002294, for $K = 6$, …, in the online Encyclopedia of Integer Sequences [**16**].

2. Molecular species and molecular expansion

A *molecular species* M is a species having only one isomorphy type. In other words, any two M-structures are isomorphic. A molecular species M is characterized by its *degree*, n (the size of the underlying set of any M-structure) and by the *stabilizer* H of any M-structure s on $[n] = \{1, 2, \ldots, n\}$, that is the subgroup of the symmetric group $\mathbb{S}_n$, consisting of all automorphisms of s. More precisely, two molecular species M and M' of degree n are equal if and only if the stabilizers H and H' (resp.) are conjugate subgroups of $\mathbb{S}_n$.

Here are some examples of molecular species:

- $M = E_n$, the species of *sets* of size n ($n \geq 0$), where the stabilizer group H is $\mathbb{S}_n$, with $E_0 = 1$ and $E_1 = X$;
- $M = X^n$, the species of *n-lists* or *linear orders* of length n ($n \geq 0$), where $H = 1$;
- $M = C_n$, the species of *oriented cycles* of length n ($n \geq 1$), where $H = <\rho>$, the subgroup of $\mathbb{S}_n$ generated by the circular permutation (rotation) $\rho = (1, 2, \ldots, n)$, with $C_1 = X$ and $C_2 = E_2$;
- $M = P_n$, the species of *polygons* (unoriented cycles) of size n ($n \geq 3$), where $H = D_n$, the dihedral group of degree n (and order $2n$) generated by the rotation $\rho = (1, 2, \ldots, n)$ and the reflection $\tau = (1, n)(2, n-1)\cdots$, with $P_3 = E_3$.

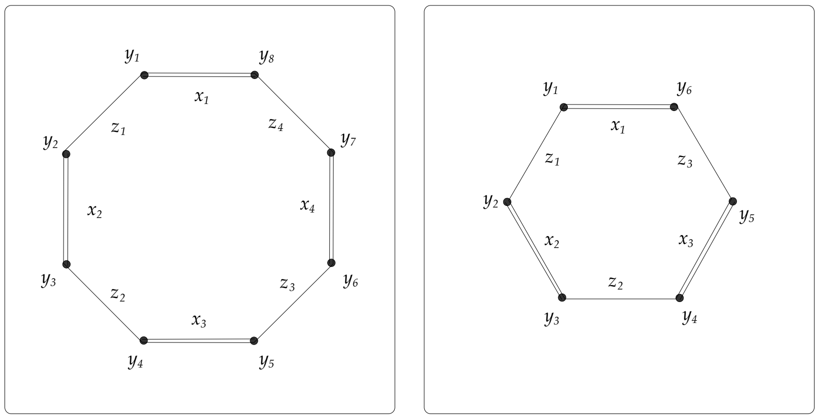
For more information on molecular species, see [**1, 11**]. We denote by

$$\mathcal{M} = \{1,\ X,\ X^2,\ E_2,\ X^3,\ XE_2,\ E_3,\ C_3,\ \ldots\}, \tag{2.1}$$

the set of all molecular species. Any species F can be expressed as a (possibly infinite) linear combination with integer coefficients of molecular species as follows:

$$F = \sum_{M\in\mathcal{M}} f_M M, \tag{2.2}$$

where $f_M \in \mathbb{N}$ represents the number of molecular subspecies of F isomorphic to M. This expansion is unique and is called the *molecular expansion* of the species F. Our goal is to determine an expansion of the form (2.2) for the species $\mathfrak{a}$ of outerplanar K-gonal 2-trees for general $K \geq 3$, extending previous work [**11**] for $K = 3$.



a) b)

FIGURE 3. a) A $P_8^{\mathrm{bic}}(X,Y,Z)$-structure and b) a $P_6^{\mathrm{bic}}(X,Y,Z)$-structure

2.1. Bicolored polygons. Let $P_{2n}^{\mathrm{bic}}(X,Y,Z)$ denote the three-sort species of bicolored $2n$-gons, $n \geq 2$. More precisely, we consider polygons with $2n$ vertices, of sort Y, where the edges are colored with two colors $\{0,1\}$, in such a way that incident edges have different colors, and the sorts X and Z are associated to edges colored 0 and 1, respectively. Figure 3 represents $P_{2n}^{\mathrm{bic}}(X,Y,Z)$-structures for $n=4$ and $n=3$. The double edges, of sort X, correspond to the color 0 and the single edges, of sort Z, to the color 1. The stabilizer H of a $P_{2n}^{\mathrm{bic}}(X,Y,Z)$-structure is a subgroup of the symmetric group $\mathbb{S}_n^X \times \mathbb{S}_{2n}^Y \times \mathbb{S}_n^Z$, isomorphic to the dihedral group D_n, generated by a rotation ρ and a reflection τ:

$$\rho = (y_1, y_3, \ldots, y_{2n-1})(y_2, y_4, \ldots, y_{2n})(x_1, x_2, \ldots, x_n)(z_1, z_2, \ldots, z_n)$$

and

$$\tau = (y_1, y_{2n})(y_2, y_{2n-1}) \cdots (y_n, y_{n+1})(x_1)(x_2, x_n) \cdots (z_1, z_n) \cdots .$$

One-sort and two-sort species of bicolored polygons have been considered before; see [**14, 11**]. In particular, we have

$$P_{2n}^{\mathrm{bic}}(X,Y) = P_{2n}^{\mathrm{bic}}(X,Y,1) \qquad \text{and} \qquad P_{2n}^{\mathrm{bic}}(Y) = P_{2n}^{\mathrm{bic}}(1,Y,1)$$

where setting a sort $X := 1$ in a species means that the elements of sort X are unlabelled. Also notice that for the species P_n of (usual) polygons we have the identifications

$$P_n(X) = P_{2n}^{\mathrm{bic}}(X,1,1) = P_{2n}^{\mathrm{bic}}(1,1,X).$$

By convention we also define

$$P_2^{\mathrm{bic}}(X,Y,Z) := XZE_2(Y).$$

Bicolored polygons are naturally related to outerplanar K-gonal 2-trees having a dihedral symmetry. For instance, in Figure 4, we see two identifications of bicolored polygons with outerplanar triangular 2-trees. In these identifications, the $2n$ vertices become oriented edges for which oriented-edge rooted 2-trees can be substituted.

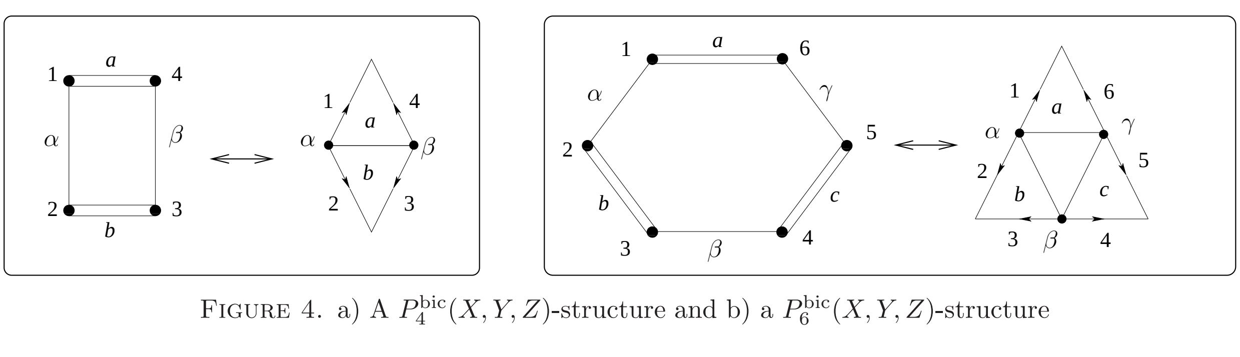


FIGURE 4. a) A $P_4^{\mathrm{bic}}(X,Y,Z)$-structure and b) a $P_6^{\mathrm{bic}}(X,Y,Z)$-structure

2.2. Addition formulas. Let us recall from [**11**] two addition formulas relative to the species E_2 of two-element sets and $P_4^{\mathrm{bic}}(X,Y)$ of bicolored quadrilaterals. These are used in the computation of the molecular expansions of the species a^- and $a^{\hat{\diamond}}$. Let $B = B(Y)$ denote any asymmetric species, with molecular expansion

$$B(Y) = \sum_{m\geq 0} b_m Y^m, \quad b_m \in \mathbb{N}\,.$$

Let $b_m^{(j)}$ denote the coefficient of Y^m in the species $B^j(Y)$. We make the convention that $b_x^{(j)} = 0$ if the index x is fractional.

Proposition 2.1 ([**11**]). *We have*

$$E_2(B(Y)) = \sum_{m\geq 1} b_m E_2(Y^m) + \sum_{m\geq 0} e_m Y^m, \tag{2.3}$$

where

$$e_0 = \frac{1}{2}(b_0^2 + b_0) \quad \textit{and} \quad e_m = \frac{1}{2}(b_m^{(2)} - b_{\frac{m}{2}}), \quad m \geq 1\ . \tag{2.4}$$

□

Proposition 2.2 ([**11**]). *We have*

$$P_4^{\mathrm{bic}}(X,B(Y)) = \sum_{m\geq 1} \beta_m^{'} X^2 Y^m + \sum_{m\geq 1} \beta_m^{''} E_2(XY^m) + \sum_{m\geq 1} \beta_m^{'''} X^2 E_2(Y^m) + \sum_{m\geq 0} \beta_m^{iv} P_4^{\mathrm{bic}}(X,Y^m), \tag{2.5}$$

where

$$\beta_m^{'} = \frac{1}{4}b_m^{(4)} - \frac{3}{4}b_{\frac{m}{2}}^{(2)} + \frac{1}{2}b_{\frac{m}{4}}, \quad \beta_m^{''} = b_m^{(2)} - b_{\frac{m}{2}}, \quad \beta_m^{'''} = \frac{1}{2}(b_m^{(2)} - b_{\frac{m}{2}}) \quad \textit{and} \quad \beta_m^{iv} = b_m. \tag{2.6}$$

□

3. Dihedral classes of words over a weighted involutional alphabet $\mathcal{A}$

In order to classify $a^{\diamond}$-structures, that is polygon-rooted outerplanar K-gonal 2-trees, we consider them as equivalence classes of oriented cycles of A-structures under reflection or, more precisely, as equivalence classes of words under conjugation and reflection (called *dihedral classes* of words) in an alphabet $\mathcal{A}$ constituted by the (unlabelled) A-structures themselves. Thus a letter $a \in \mathcal{A}$ is an isomorphism type of oriented-external-edge rooted outerplanar K-gonal 2-trees.

The alphabet $\mathcal{A}$ is weighted as follows. We define the *weight* of a letter $a \in \mathcal{A}$ as X^n if a is of degree n and the *weight* of a word in $\mathcal{A}^*$ as the product of the weights of its letters. Moreover, the alphabet is involutional in the following sense: there is an involutive operator $a \mapsto \overline{a}$ where $\overline{a}$ denotes the *opposite* letter, associated to the isomorphy type obtained from a by reversing the orientation of its root-edge. For any word $w = a_1 \cdots a_n \in \mathcal{A}^*$, the *opposite* word of w, denoted $\overline{w}$ is defined by $\overline{w} = \overline{a_n} \cdots \overline{a_1}$.

The dihedral group $D_n = \langle \rho, \tau \rangle$ acts on the set of words of length n over $\mathcal{A}$ as follows: for a word $w = a_1\ a_2 \cdots a_n$, we have

$$\rho \cdot w = a_n\ a_1\ a_2 \ldots a_{n-1} \qquad \text{and} \qquad \tau \cdot w = \overline{w}.$$

The *circular class* of a word $w \in \mathcal{A}^*$, denoted by $[w]$, is defined as the orbit of w under the action of $\langle \rho \rangle$. The *dihedral class* of a word $w \in \mathcal{A}^*$, denoted by $[[w]]$, is defined as the orbit of w under the action of D_n. Notice that $[[w]] = [w] \cup [\overline{w}]$. Also, the weight of a word is preserved under the action of ρ and of τ so that the *weight* of a circular or dihedral class can be defined as the weight of any word in the class.

A word $w \in \mathcal{A}^*$ is called a *palindrome* if $w = \overline{w}$. A word $w \in \mathcal{A}^*$ is called a *dexterpalindrome* if it is the concatenation of a τ-symmetric letter a (that is, $\overline{a} = a$) followed by a palindrome. If a word w is a palindrome or a dexterpalindrome then the circular classes of w and $\overline{w}$ coincide: $[w] = [\overline{w}] = [[w]]$. On the other hand, if $[w] \neq [\overline{w}]$, the word w is called *skew*; the circular class $[w]$ is also called *skew*. A dihedral or circular class is called *palindromic* (resp. *dexterpalindromic*) if it contains a palindrome (resp. a dexterpalindrome). A word is said to be *primitive* if it is not a power of another word. A circular class $[w]$ or a dihedral class $[[w]]$ is called *primitive* if the word w is primitive. We now wish to enumerate these classes of words. We set

$\lambda(d,m) =$ the number of primitive circular classes of words of length d and weight X^m;

$\Pi(d,m) =$ the number of primitive palindromic words of length d and weight X^m;

$\pi(d,m) =$ the number of primitive palindromic dihedral classes of words of length d and weight X^m;
$\delta(d,m) =$ the number of primitive dexterpalindromic dihedral classes of length d and weight X^m;
$\sigma(d,m) =$ the number of primitive skew circular classes of words of length d and weight X^m.

Classifying words according to their primitive roots and using Möbius inversion, we obtain the following.

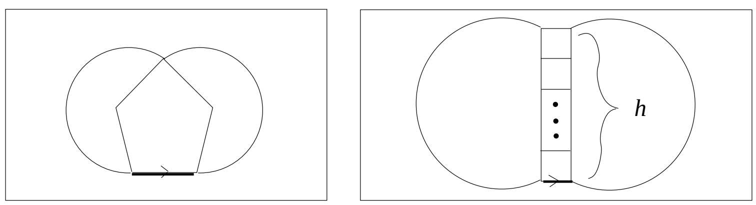
PROPOSITION 3.1. *Let $d \in \mathbb{N}$. Then, we have*

$$a_m^{(d)} = \sum_{ij=d} i\,\lambda(i, m/j), \tag{3.1}$$

$$\lambda(d,m) = \frac{1}{d}\sum_{ij=d} \mu(j) a_{m/j}^{(i)}. \tag{3.2}$$

□

If w is a palindrome of odd length d in the alphabet $\mathcal{A}$, then its central letter a is τ-symmetric. This means that the isomorphism type corresponding to a is itself τ-symmetric that is, invariant under an orientation reversal of its root-edge. We define the *height* h of a τ-symmetric letter a to be the number of K-gons located directly above its root edge. Note that if K is odd, the height can only be 0 or 1. See Figure 5.



a) b)

FIGURE 5. τ-symmetric structures, a) K odd b) K even

Let d be an odd integer and let $\mathrm{Pal}(d,h,m)$ denote the set of palindromes w of length d, of weight X^m, and such that the central letter is of height h. We set

$\mathrm{pal}(d,h,m) = |\mathrm{Pal}(d,h,m)|$;
$\pi(d,h,m) =$ the number of primitive palindromic dihedral classes of words $w \in \mathrm{Pal}(d,h,m)$.

PROPOSITION 3.2. *Let d be an odd integer. Then, for K odd, and $h = 0$ or 1, we have*

$$\mathrm{pal}(d,h,m) = [X^{\frac{m-h}{2}}]\; A^{h\frac{K-1}{2}+\frac{d-1}{2}} = a_{\frac{m-h}{2}}^{(h\frac{K-1}{2}+\frac{d-1}{2})} \tag{3.3}$$

while, for K even and $h = 0,\ldots,m$, we have

$$\mathrm{pal}(d,h,m) = [X^{\frac{m-h}{2}}]\; A^{h\frac{K-2}{2}+\frac{d-1}{2}} = a_{\frac{m-h}{2}}^{(h\frac{K-2}{2}+\frac{d-1}{2})}. \tag{3.4}$$

□

PROPOSITION 3.3. *Let d be an odd integer. Then,*

$$\mathrm{pal}(d,h,m) = \sum_{ij=d} \pi(i,h,m/j), \tag{3.5}$$

$$\pi(d,h,m) = \sum_{ij=d} \mu(j)\,\mathrm{pal}(i,h,m/j), \tag{3.6}$$

where μ denotes the Möbius function.

PROOF. These relations follow from the fact that a primitive palindromic class of odd length contains exactly one palindrome and from Möbius inversion. ■

3.1. Case K odd. We now assume K is odd. The next proposition is readily established.

Proposition 3.4. *Let d be an odd integer. Then*

$$\pi(d,m) = \sum_{n\geq 0} \pi(d,n,m), \tag{3.7}$$

$$\sigma(d,m) = \frac{1}{2}(\lambda(d,m) - \pi(d,m)). \tag{3.8}$$

□

3.2. Case K even. We now assume that K is even.

Proposition 3.5. *We have*

$$\mathrm{pal}(d,m) = \begin{cases} a_{\frac{m}{2}}^{(\frac{d}{2})}, & \textit{if } d \textit{ is even}, \\ \sum_{h\geq 0} \mathrm{pal}(d,h,m), & \textit{if } d \textit{ is odd}. \end{cases} \tag{3.9}$$

□

Proposition 3.6. *We have*

$$\mathrm{pal}(d,m) = \sum_{ij=d} \Pi(i, m/j), \tag{3.10}$$

$$\Pi(d,m) = \sum_{ij=d} \mu(j)\mathrm{pal}(i, m/j), \tag{3.11}$$

$$\pi(d,m) = \frac{1}{1+\chi(d \text{ is even})}\Pi(d,m). \tag{3.12}$$

□

Let d be a positive integer and let $\mathrm{Dext}(d,h,m)$ denote the set of dexterpalindromes aw of length d, of weight X^m, and such that the first letter, a, is of height h. We set

$\mathrm{dext}(d,h,m) = |\mathrm{Dext}(d,h,m)|$;

$\Delta(d,h,m) =$ the number of primitive dexterpalindromes in $\mathrm{Dext}(d,h,m)$;

$\delta(d,h,m) =$ the number of primitive dexterpalindromic dihedral classes of words in $\mathrm{Dext}(d,h,m)$.

Proposition 3.7. *We have*

$$\mathrm{dext}(d,h,m) = \sum_{\substack{n\geq 0,\, h\geq 0\\ 2n+h\leq m}} a_n^{(h\frac{K-2}{2})}\mathrm{pal}(d-1,\, m-2n-h), \tag{3.13}$$

$$\mathrm{dext}(d,h,m) = \sum_{ij=d} \Delta(i,h,m/j), \tag{3.14}$$

$$\Delta(d,h,m) = \sum_{ij=d} \mu(j)\,\mathrm{dext}(i,h,m/j). \tag{3.15}$$

□

Let d be a positive even integer and let $\mathrm{Dext}(d,h_1,h_2,m)$ denote the set of dexterpalindromes aw of length d, of weight X^m, and such that the first letter, a, is of height h_1 and the central letter of w is of height h_2. We set

$\mathrm{dext}(d,h_1,h_2,m) = |\mathrm{Dext}(d,h_1,h_2,m)|$;

$\Delta(d,h_1,h_2,m) =$ the number of primitive dexterpalindromes in $\mathrm{Dext}(d,h_1,h_2,m)$;

$\delta(d,h_1,h_2,m) =$ the number of primitive dexterpalindromic dihedral classes of words in $\mathrm{Dext}(d,h_1,h_2,m)$.

Proposition 3.8. *Let d be an even positive integer and h_1, h_2 be non-negative integers. Then, we have*

$$\mathrm{Dext}(d,h_1,h_2,m) = [X^{\frac{m-h_1-h_2}{2}}]A^{\frac{K-2}{2}(h_1+h_2)+\frac{d-2}{2}} = a_{\frac{m-h_1-h_2}{2}}^{(\frac{K-2}{2}(h_1+h_2)+\frac{d-2}{2})}. \tag{3.16}$$

□

PROPOSITION 3.9. *Let d be an even positive integer and h_1, h_2 be non-negative integers such that $h_1 \neq h_2$. Then,*

$$\begin{aligned} \mathrm{Dext}(d, h_1, h_2, m) &= \sum_{ij=d,\, j \,\mathrm{odd}} \mathrm{dext}(i, h_1, h_2, m/j), & (3.17)\\ \mathrm{dext}(d, h_1, h_2, m) &= \delta(d, h_1, h_2, m) = \sum_{ij=d,\, j \,\mathrm{odd}} \mu(j) \mathrm{Dext}(i, h_1, h_2, m/j). & (3.18)\end{aligned}$$

PROPOSITION 3.10. *Let d be an even positive integer and n a non-negative integer. Then we have*

$$\begin{aligned} \mathrm{Dext}(d, n, n, m) &= \sum_{ij=d,\, j \,\mathrm{odd}} \Delta(i, n, n, m/j) + \sum_{ij=d,\, j \,\mathrm{even}} \Delta(i, n, m/j), & (3.19)\\ \Delta(d, n, n, m) &= \sum_{ij=d,\, j \,\mathrm{odd}} \mu(j) \Big(\mathrm{Dext}(i, n, n, m/j) - \sum_{\ell k=i,\, k \,\mathrm{even}} \Delta(\ell, n, \frac{m}{jk}) \Big), & (3.20)\\ \delta(d, n, n, m) &= \frac{1}{2} \Delta(d, n, n, m). & (3.21)\end{aligned}$$

PROPOSITION 3.11. *Let d be an even integer. Then, we have*

$$\delta(d, m) = \sum_{h_1 \geq 0} \sum_{h_2 \geq h_1} \delta(d, h_1, h_2, m). \quad (3.22)$$

□

PROPOSITION 3.12. *Let d be a positive integer. Then,*

$$\sigma(d, m) = \frac{1}{2} \left(\lambda(d, m) - \pi(d, m) - \chi(d \text{ even}) \, \delta(d, m) \right). \quad (3.23)$$

□

4. The molecular expansion of a

4.1. The molecular expansion when K is odd. Let $K \geq 3$ be an odd integer. In this section, we obtain the molecular expansion of the species a of outerplanar K-gonal 2-trees.We begin by expressing a^- and $a^{\triangle}$ in terms of the species E_2, P_4^{bic} and A. The addition formulas given in Section 2.2 can then be used to give their molecular expansions.

THEOREM 4.1. *If K is odd, then the species a^- and $a^{\triangle}$ of outerplanar K-gonal 2-trees pointed at an edge and at a K-gon with a distinguished edge, respectively, are given in terms of the species A by*

$$\begin{aligned} a^- &= 1 + X E_2(A^{\frac{K-1}{2}}) + P_4^{\mathrm{bic}}(X, A^{\frac{K-1}{2}}), & (4.1)\\ a^{\triangle} &= X E_2(A^{\frac{K-1}{2}}) + X^2 E_2(A^{K-1}). & (4.2)\end{aligned}$$

PROOF. The proof is analogous to the case where $K = 3$. See [**11**] and Figure 6, where $K = 5$. ■

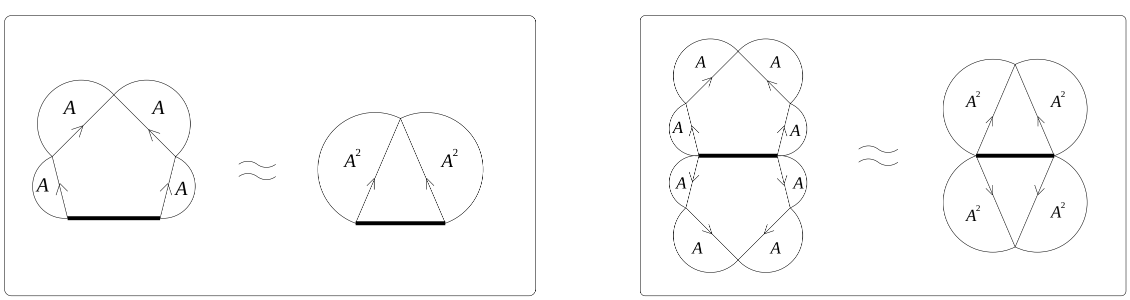


FIGURE 6. Description of the species a^- in terms of outerplanar triangular 2-trees

THEOREM 4.2. *If K is odd, then the molecular expansion of the species $\mathfrak{a}^{\diamond}$ of outerplanar K-gonal 2-trees rooted at a K-gon is given by*

$$\mathfrak{a}^{\diamond} = \sum_{m\geq 0}\sum_{d|K} \pi(d,0,2m) X P^{\mathrm{bic}}_{\frac{2K}{d}}(1,X^m,1) + \sum_{m\geq 0}\sum_{d|K} \pi(d,1,2m+1) X P^{\mathrm{bic}}_{\frac{2K}{d}}(X,X^m,1) \tag{4.3}$$

$$+ \sum_{m\geq 0}\sum_{d|K} \sigma(d,m) X C_{\frac{K}{d}}(X^m). \tag{4.4}$$

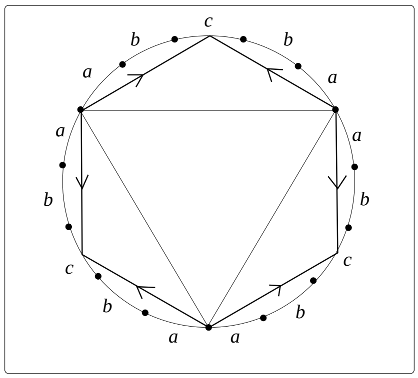


FIGURE 7. An $\mathfrak{a}^{\diamond}$-structure, with $K = 15$

PROOF. We classify the $\mathfrak{a}^{\diamond}$-structures according to the dihedral classes of words in $\mathcal{A}$ that they determine and to the length d of their primitive roots. If the class is palindromic, as in Figure 7, we obtain a $P^{\mathrm{bic}}_{\frac{2K}{d}}$-structure while if the class is skew, we obtain a $C_{\frac{K}{d}}$-structure. ∎

Finally, putting together the molecular expansion of the species $\mathfrak{a}^{-}$, $\mathfrak{a}^{\hat{\diamond}}$ and $\mathfrak{a}^{\diamond}$, and using the Dissymmetry theorem, we obtain the molecular expansion of the species $\mathfrak{a}$ of outerplanar K-gonal 2-trees.

THEOREM 4.3. *Let $K \geq 3$ be an odd integer. Then, the molecular expansion of the species $\mathfrak{a}$ of outerplanar K-gonal 2-trees is given by*

$$\mathfrak{a} = \sum_{m\geq 3} \alpha_m X^m + \sum_{m\geq 2} \beta_m E_2(X^m) + \sum_{m\geq 2} \gamma_m X E_2(X^m) + \sum_{m\geq 1} \delta_m X^2 E_2(X^m) \tag{4.5}$$

$$+ \sum_{m\geq 0} \varepsilon_m P^{\mathrm{bic}}_4(X,X^m,1) + \sum_{h=0}^{1}\sum_{m\geq 0}\sum_{\substack{d|K\\ d<K}} \pi(d,h,2m+n) X P^{\mathrm{bic}}_{\frac{2K}{d}}(X^n,X^m,1) \tag{4.6}$$

$$+ \sum_{m\geq 0}\sum_{\substack{d|K\\ d<K}} \sigma(d,m) X C_{\frac{K}{d}}(X^m), \tag{4.7}$$

with

$$\alpha_m = \sigma(K,m-1) + \frac{1}{2} a^{(\frac{K-1}{2})}_{\frac{m-2}{4}} - \frac{1}{4}\left(a^{(2K-2)}_{m-2} + a^{(K-1)}_{\frac{m-2}{2}}\right), \tag{4.8}$$

$$\beta_m = a^{(K-1)}_{m-1} - a^{(\frac{K-1}{2})}_{\frac{m-1}{2}}, \tag{4.9}$$

$$\gamma_m = \pi(K,0,2m), \tag{4.10}$$

$$\delta_m = \pi(K,1,2m+1) - \frac{1}{2}\left(a^{(K-1)}_m + a^{(\frac{K-1}{2})}_{\frac{m}{2}}\right), \tag{4.11}$$

$$\varepsilon_m = a^{(\frac{K-1}{2})}_m. \tag{4.12}$$

□

4.2. Molecular expansions when K is even.

THEOREM 4.4. *Let $K \geq 4$ be any even integer. The species a^- and $a^{\diamond\!\!-}$ of outerplanar K-gonal 2-trees pointed at an edge and at a K-gon with a distinguished edge, respectively, are given in terms of the species A by*

$$a^- = 1 + \sum_{n\geq 1} \left\lceil \frac{n}{2} \right\rceil X^n E_2(A^{n\frac{K-2}{2}}) + \sum_{\substack{n\geq 2\\ n \text{ even}}} P_4^{\text{bic}}(X^{\frac{n}{2}}, A^{n\frac{K-2}{4}}), \tag{4.13}$$

$$a^{\diamond\!\!-} = \sum_{n\geq 1} n\, X^n E_2(A^{n\frac{K-2}{2}}), \tag{4.14}$$

where $\lceil\cdot\rceil$ is the ceiling function.

PROOF. We begin with the species a^- of edge-pointed K-gonal 2-trees. We classify its structures according to the number n of K-gons located directly above or below their root edge. These K-gons form the *ladder* of the structure. The 1 in equation (4.13) stands for the single edge ($n = 0$). Next, we consider the possible positions of the root-edge on the ladder. There are $\lceil \frac{n}{2} \rceil$ non-central positions (see Figure 8 a)) which are of isomorphy type $X^n E_2(A^{n\frac{K-2}{2}})$. This yields the second term of (4.13). If the root edge stands in the center

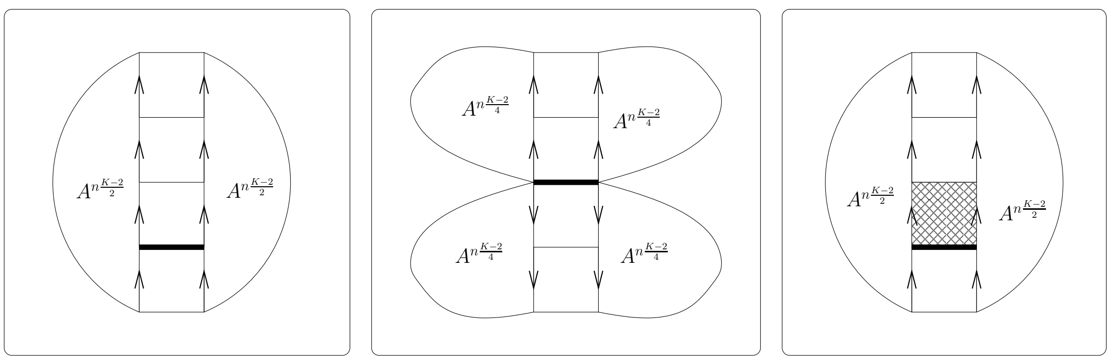


FIGURE 8. a)–b) the species a^-, c) the species $a^{\diamond\!\!-}$

of the ladder, as in Figure 8 b), the isomorphy type corresponds to the species $P_4^{\text{bic}}(X^{\frac{n}{2}}, A^{\frac{n}{2}\frac{K-2}{2}})$, giving the third term of (4.13). Relation (4.14) is obtained in a similar way. ∎

Making use of the addition formulas of Section 2.2, the molecular expansion of the species a^- and $a^{\diamond\!\!-}$ can be obtained in a straightforward way.

THEOREM 4.5. *Let $K \geq 4$ be any even integer. Then, the molecular expansion of the species $a^\diamond$ of outerplanar K-gonal 2-trees pointed at a K-gon is given by*

$$a^\diamond = \sum_{h\geq 0}\sum_{m\geq 0}\sum_{\substack{d|K\\ d \text{ odd}}} \pi(d,h,2m+h)\, X\, P^{\text{bic}}_{\frac{2K}{d}}(X^h, X^m, 1) \tag{4.15}$$

$$+ \sum_{n\geq 1}\sum_{\substack{d|K\\ d \text{ even}}} \pi(d,2n)\, X\, P^{\text{bic}}_{\frac{2K}{d}}(1, X^n, 1) \tag{4.16}$$

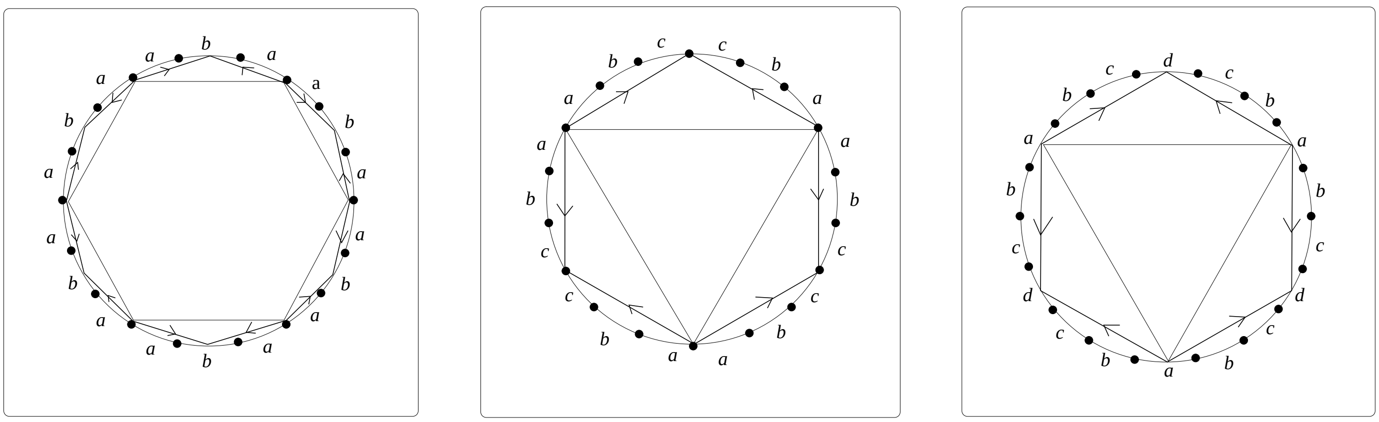
$$+ \sum_{\ell\geq 0}\sum_{m\geq \ell}\sum_{n\geq 0}\sum_{\substack{d|K\\ d \text{ even}}} \delta(d,\ell,m,2n+\ell+m)\, X\, P^{\text{bic}}_{\frac{2K}{d}}(X^\ell, X^n, X^m) \tag{4.17}$$

$$+ \sum_{m\geq 2}\sum_{d|K} \sigma(d,m)\, X\, C_{\frac{K}{d}}(X^m). \tag{4.18}$$

PROOF. Again, we classify the $a^\diamond$-structures according to the dihedral classes of words $[[w]]$ in $\mathcal{A}$ that they determine and to the length d of their primitive roots r. Three different cases can occur: $[[w]]$ can be palindromic, dexterpalindromic or skew.

If $[[w]]$ is palindromic, then if d is odd, as illustrated by Figure 9 a), with $r = ab\overline{a}$, $b = \overline{b}$, then the central letter of r is symmetric of height h and we get the first term of (4.15) and if d is even, as illustrated by Figure 9 b), with $r = abc\overline{c}\overline{b}a$, we obtain the term (4.16).

If $[[w]]$ is dexterpalindromic as in Figure 9 c), where $r = abcd\overline{c}\overline{b}$ such that $a = \overline{a}$ and $d = \overline{d}$, the heights of a and d being equal to ℓ and m respectively, we obtain the term (4.17). Finally, if $[[w]]$ is skew, we get (4.18). ■



a) b) c)

FIGURE 9. Some $\mathfrak{a}^{\diamond}$-structures, with $K = 18$

We are now able to give the final result of the present paper, that is, the molecular expansion of the species of outerplanar K-gonal 2-trees, for an even integer K.

THEOREM 4.6. *Let $K \geq 4$ be any even integer. Then, the molecular expansion of the species $\mathfrak{a}$ of outerplanar K-gonal 2-trees is given by*

$$\mathfrak{a} = 1 + \sum_{m\geq 1} \alpha_m X^m + \sum_{m\geq 1} \beta_m E_2(X^m) \tag{4.19}$$

$$+ \sum_{m\geq 1}\sum_{n\geq 1} \gamma_{m,n} X^n E_2(X^m) + \sum_{m\geq 1}\sum_{n\geq 1} \delta_{m,n} X^{2n} E_2(X^m)$$

$$+ \sum_{m\geq 0}\sum_{n\geq 1} \varepsilon_{m,n} P_4^{\mathrm{bic}}(X^n, X^m, 1), \tag{4.20}$$

$$+ \sum_{h\geq 0}\sum_{m\geq 0}\sum_{\substack{d|K \\ d \text{ odd}}} \pi(d, h, 2m+h)\, X\, P^{\mathrm{bic}}_{\frac{2K}{d}}(X^h, X^m, 1)$$

$$+ \sum_{n\geq 0}\sum_{\substack{d|K \\ d \text{ even}}} \pi(d, 2n)\, X\, P^{\mathrm{bic}}_{\frac{2K}{d}}(1, X^n, 1) \tag{4.21}$$

$$+ \sum_{\ell\geq 0}\sum_{m\geq \ell}\sum_{n\geq 0}\sum_{\substack{d|K,\ d<K \\ d \text{ even}}} \delta(d, \ell, m, 2n+\ell+m)\, X\, P^{\mathrm{bic}}_{\frac{2K}{d}}(X^\ell, X^n, X^m) \tag{4.22}$$

$$+ \sum_{m\geq 2}\sum_{\substack{d|K \\ d<K/2}} \sigma(d, m)\, X\, C_{\frac{K}{d}}(X^m), \tag{4.23}$$

where

$$\begin{aligned}
\alpha_m &= \sigma(K,m-1) - \sum_{n\geq 1}\frac{\lfloor n/2\rfloor}{2}\left(a_{m-n}^{(n(K-2))} - a_{\frac{m-n}{2}}^{(n\frac{K-2}{2})}\right) - \frac{1}{4}a_{m-2n}^{(2n(K-2))} + \frac{3}{4}a_{\frac{m-2n}{2}}^{(n(K-2))} - \frac{1}{2}a_{\frac{m-2n}{4}}^{(n\frac{K-2}{2})},\\
\beta_m &= \sum_{n\geq 1} a_{m-n}^{(n(K-2))} - a_{\frac{m-n}{2}}^{(n\frac{K-2}{2})},\\
\gamma_{m,n} &= \sum_{i=0}^{\lfloor\frac{n}{2}\rfloor}\delta(K,i,n-i,2m+n) + \chi(n=1)\sigma(\frac{K}{2},m) - \left\lfloor\frac{n}{2}\right\rfloor a_m^{(n\frac{K-2}{2})},\\
\delta_{m,n} &= \frac{1}{2}(a_m^{(n(K-2))} - a_{\frac{m}{2}}^{(n\frac{K-2}{2})}),\\
\varepsilon_{m,n} &= a_m^{(n\frac{K-2}{2})}.
\end{aligned}$$

□

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