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ORIGINAL PAPER

Enumerating stereo-isomers of tree-like polyinositols

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Abstract Enumeration of molecules is one of the fundamental problems in bioinformatics and chemoinformatics which is also important from a practical viewpoint. We consider the problem of enumerating the stereo-isomers of tree-like polyinositol molecules (with chemical formula $C_{6n}O_{5n+6}H_{4n+2}$ where n is the number of hexagonal oinositol rings) and monosubstituted tree-like polyinositols (with chemical formula $C_{6n}O_{5n+6}H_{4n+1}Z$). We establish recursion counting formulas for the numbers of the stereo-isomers for these two classes of molecules, in which chirality is also taken into account. In our study, the generating function, Pólya enumeration theory and 'Dissimilarity Characteristic Theorem' play important roles. Compared to some known computer programs such as ISOMERS, MOLGEN, exhaustive construction and Dynamic Programming etc., our method is more efficient to our enumeration problem with larger number of inositol rings. Further more, based on the obtained recursion formulas, we derive the asymptotic values for the numbers of these two stereo-isomers from which we conclude that almost all tree-like and monosubstituted tree-like polyinositols are chiral.

Keywords Tree-like polyinositol · Enumeration · Asymptotic behavior

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1 Introduction

Enumeration of molecules is one of the fundamental problems in bioinformatics, chemoinformatics and has attracted chemists, biologists and mathematicians for more than one century [1,2]. It is also important from a practical viewpoint because it plays an important role in drug discovery, experimental structure elucidation, molecular design [3], virtual libraries constructing, hypotheses testing and experiments optimizing [4].

We consider the enumeration problem of the stereo-isomers of tree-like polyinositol (TL-polyinositol) molecules. A TL-polyinositol (with chemical formula $C_{6n}O_{5n+6}H_{4n+2}$) molecule is a three-dimensional polymer, consisting of n hexagonal inositol rings (a six carbon ring structure with a hydrogen and a hydroxyl group at each carbon position), any two of which are connected by at most one C–O–C bond and whose planar chemical graph will tend into a tree after contracting each inositol ring into a vertex, see Fig. 1. Because of the rapid inter-conversion of conformers, each inositol ring can be schematized by a planar hexagon. The C–H bond and the C–O bond at the same carbon position lie on different sides of the planar hexagon, i.e., one is above the horizontal planar hexagon while the other is below, if we fix the planar hexagon in the average plane.

Of the lowest weight among TL-polyinositols, inositol or cyclohexane-1, 2, 3, 4, 5, 6- hexol [5,6] exists in nine (when chirality is ignored) possible stereo-isomers [7], of which the most prominent form and widely occurring in nature, is myo-inositol (former name meso-inositol), see Fig. 1a. The synthesis and properties of inositols have been widely studied by chemists [8–13]. Many other oligomers of TL-polyinositols i.e., oligoinositols, have also been synthesized and studied, such as the linear polyinositols 1,2-L-chiro-inositol conjugates [14] which suggest a tendency towards a β-3-turn secondary structure; muco-inositols [15] whose properties and biological activities were investigated; and others [16] whose biological evaluations were studied by being tested against some glycosidase and by NMR experiments.

Enumerating tree-like molecules or acyclic chemical compounds may date from 1857 when Cayley [1] successfully found a recursive formula for the number of alkanes. In the past few decades, various techniques were established for enumerating tree-like molecules [17–20]. And lots of tree-like molecules beyond alkanes have been discussed, e.g., tree-like polyhexes (with asymptotic analysis) [21]; phenylenes [22]; tree-like polymer [23]; radicals, monoalcohols, glycols and esters [24]; aliphatic cyclopropane derivatives [25], etc. In mathematical aspects, a large number of trees or tree-like graphs with some specific requirements were also discussed; we refer to [26–34] and the references cited therein, for examples.

In general, it is difficult to get an explicit expression for the number of tree-like configurations. Instead, finding a recursion counting formula to deal with the problem has been shown to be an effective approach. When a recursion formula is established, its asymptotic behavior is analyzed as well. Pólya [2] and Otter's [18] methodology for analyzing the asymptotic behavior was systematically summarized by Harary et al [19], as the so-called 'twenty-step algorithm'.

We note that in the above enumeration problems, all the molecules are modeled, in terms of graph theory, as unlabeled trees. In practice, however, some enumeration

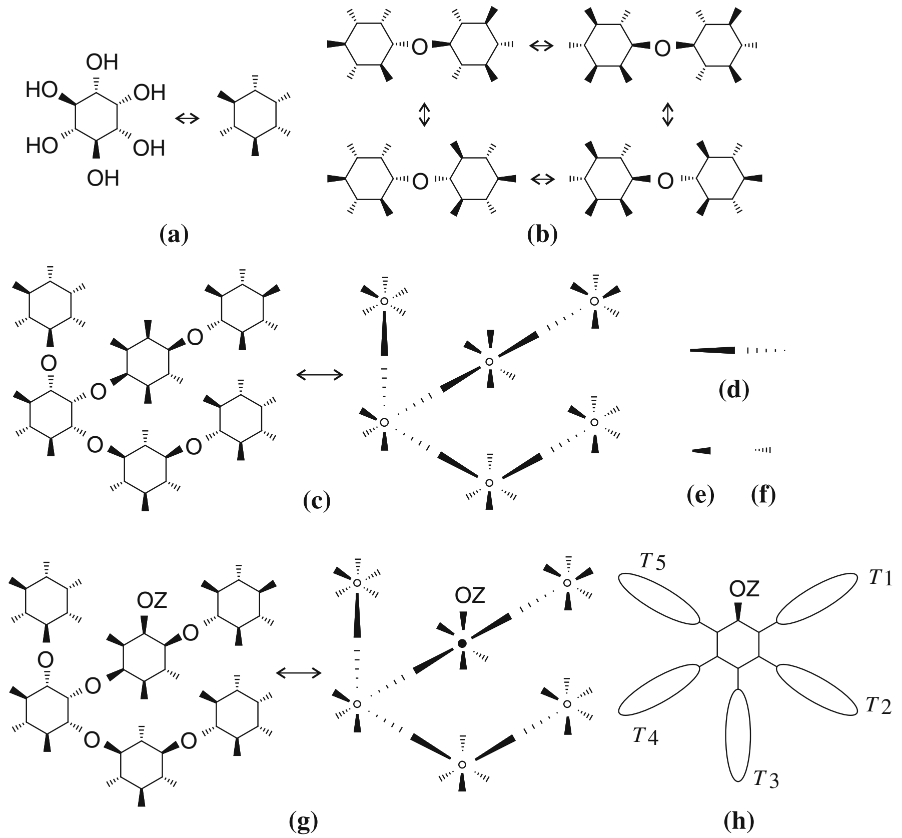

Fig. 1 **a** Molecule graph for myo-inositol. The –H is omitted in each C–H bond. The *black and dashed lines* represent that the corresponding C–O bonds are above and below the incident inositol ring, respectively. **b** The four equivalent molecule graphs of a diinositol. **c** A tree-like polyinositol (*left*) and its contracted tree (*right*). **d**. A long edge. **e** A short edge above some hexagonal plane. **f** A short edge below some hexagonal plane. **g** A monosubstituted tree-like polyinositol (*left*) and its contracted rooted tree (*right*), where the black vertex represents the planted inner vertex. **h** The general structure of a monosubstituted tree-like polyinositol in which some T_i may be an –OH group

problems in other areas are often modeled by certain kinds of labeled trees; we refer the reader to, for example, Friedberg's work [35].

The enumeration of stereo-isomers of TL-polyinositols with smaller number of inositol rings have been done by some chemists and mathematicians [36]. It was started by the question posed by Hudlicky et al [37], who wondered how many stereo-isomers exist of diinositols and of one constitutional isomer of triinositols (note that there are three constitutional isomers for triinositols). In [38] Dolhaine et al. gave the answer regarding diinositols, who obtained 528 as the number of stereo-isomers of diinositols by applying their program ISOMERS. In two subsequent papers, Dolhaine and Hönig produced the sum of the stereo-isomer numbers of all constitutional isomers of triinositols [39], and evaluated the number of possible achiral forms of some inositol tetramers [40]. And in [41], Rücker et al. counted the stereoisomers of some other oligoinositols and achiral oligoinositols, by using three methods (manual exhaustive construction, Burnside lemma and the computer program MOLGEN). They obtained the following results: (1) There are 9 monoinositols and 7 are achiral; (2) There are 528 diinositols and 48 are achiral; (3) There are 82176 triinositols with only a small fraction (768) of isomers being achiral. Recently in [3], Imada et al. enumerated the stereo-isomers of tree-like quadinositols by using Dynamic Programming.

In this paper, we aim to establish a more efficient method to count the stereo-isomers of TL-polyinositols with larger number of inositol rings, in which chirality is also taken into account. To this end, we introduce five generating functions for the numbers of TL-polyinositols and monosubstituted tree-like polyinositols (MTL-polyinositols) both in two cases (i.e., when charity is ignored and when charity is considered), and achiral MTL-polyinositols. We establish several functional equations for these generating functions by characterizing the symmetry groups caused by asymmetry around inositol rings, using Pólya's enumeration theory [2] and specifying the so-called 'Dissimilarity Characteristic theorem' [18,26] in accord with TL-polyinositols. Compared to some known computer programs such as ISOMERS, MOLGEN, exhaustive construction and Dynamic Programming etc., our method is more efficient to our enumeration problem with larger number of inositol rings. As an example, the numerical results for the number of the inositol rings up to 50 are tabulated. The above functional equations are also the fundamentals of the 'twenty-step algorithm' for analyzing the corresponding asymptotic behaviors, by which we derive the asymptotic values for the number of the corresponding stereo-isomers. The asymptotic values are well-fitting to the corresponding numerical results, from which we can conclude that almost all MTL-polyinositols and TL-polyinositols are chiral.

2 Results and discussion

2.1 Terminology and definitions

In a TL-polyinositol molecule graph, the C–OH bonds on cyclohexane rings and C–O–C bonds between cyclohexanes can be treated as rigid lines. Though there may be four kinds of rigid lines for a C–O–C bond, they can be transformed to each other by rotating one or two of its two sides [40], see Fig. 1b. Thus, to enumerate TL-polyinositol stereoisomers, we can assume that they have only straight C–O–C bonds, i.e., the C–O–C bonds in the molecular graphs in left upper and right lower position in Fig. 1b. When we contract each hexagon (inositol ring) and each OH group into a vertex, and delete –H in each C–H, the stereo molecular graph of a polyinositol will tend into a stereo rigid tree. We call it *contracted tree* of the polyinositol, see Fig. 1c. The vertices representing an OH and a hexagonal ring are called a *leaf vertex* and an *inner vertex*, respectively. The rigid lines representing a C–O–C and a C–OH bonds in a contracted tree are called a *long edge* and a *short edge*, respectively, see Fig. 1d–f.

An MTL-polyinositol is obtained from a TL-polyinositol by replacing an -OH group by a substituted group -OZ. We call this C–OZ bond and the incident hexagonal ring the *planted bond* and the *planted ring*, respectively. Consequently, we call the resulting contracted tree, the corresponding leaf vertex, incident edge and incident inner vertex the *planted contracted tree*, *planted leaf vertex*, *planted edge* and *planted inner vertex*, respectively, see Fig. 1g.

Note that our enumeration problems for TL-polyinositols and MTL-polyinositols with n hexagonal rings are now equivalent to enumerate the contracted trees and planted contracted trees with n inner vertices.

We define five generating functions involving the numbers of stereo-isomers of MTL-polyinositols and TL-polyinositols as follows, in which the prefix '(*CI*-' stands for 'when chirality is ignored', which means that each of a pair of enantiomers is separately counted, and the prefix '(*CC*-' stands for 'when chirality is considered', which means that each pair of enantiomers is counted just once.

(1). $R(x) = \sum_{n=0}^{\infty} r_n x^n$, where r_n is the number of *CI*-different MTL-polyinositols with n inositol rings;
(2). $\overline{R}(x) = \sum_{n=0}^{\infty} \overline{r}_n x^n$, where $\overline{r}_n$ is the number of *CC*-different MTL-polyinositols with n inositol rings;
(3). $T(x) = \sum_{n=1}^{\infty} t_n x^n$, where t_n is the number of *CI*-different TL-polyinositols with n inositol rings;
(4). $\overline{T}(x) = \sum_{n=1}^{\infty} \overline{t}_n x^n$, where $\overline{t}_n$ is the number of *CC*-different TL-polyinositols with n inositol rings;
(5). $B(x) = \sum_{n=0}^{\infty} b_n x^n$, where b_n is the number of achiral MTL-polyinositols.

Note 1. One can see that the number of chiral MTL-polyinositols (resp., TL-polyinositols) with n inositol rings equals to $2(r_n - \overline{r}_n)$ (resp., $2(t_n - \overline{t}_n)$), while the number of achiral MTL-polyinositols (resp., TL-polyinositols), i.e., b_n, equals to $2\overline{r}_n - r_n$ (resp., $2\overline{t}_n - t_n$).

We recall some elementary concepts of the classic Pólya's and Burnside's enumeration theory. For a permutation g of a permutation group G on an m-elements set S, it is well known that g can be split into cycles in a unique way, say b_1 cycles of length 1, b_2 cycles of length $2, \ldots, b_m$ cycles of length m ($m = b_1 + 2b_2 + \cdots + mb_m$). The cycle index of G is therefore defined by

$$P_G(x_1, x_2, \ldots, x_m) = \frac{1}{|G|} \sum_{g \in G} x_1^{b_1} x_2^{b_2} \ldots x_m^{b_m}. \tag{1}$$

A coloring $\mathcal{C}$ of S with color set C where each color c in C has a weight $w(c)$, is an assignment of each element $s \in S$ with a color $\mathcal{C}(s) \in C$. The weight of a coloring $\mathcal{C}$ (denoted by $w(\mathcal{C})$), is defined as $w(\mathcal{C}) = \sum_{s \in S} w(\mathcal{C}(s))$. Two colorings $\mathcal{C}$ and $\mathcal{C}'$ are said to be equivalent if there is a permutation $g \in G$ such that $\mathcal{C}(g(s)) = \mathcal{C}'(s)$ for any $s \in S$. Dented by z_k the number of nonequivalent colorings of S with weight k, and with

$$Z(x) = \sum_k z_k x^k,$$

as its generating function. Then by Burnside's enumeration theory,

$$z_k = \frac{1}{|G|} \sum_{g \in G} \Psi_k(g),$$

where $\Psi_k(g)$ is the number of colorings with weight k left fixed by g [42], i.e.,

$$\Psi_k(g) = |\{\mathcal{C} : w(\mathcal{C}) = k, \mathcal{C}(g(s)) = \mathcal{C}(s) \text{ for any } s \in S\}|.$$

Denote by l_w be the number of colors in C with weight w, with

$$L(x) = \sum_w l_w x^w,$$

as its the generating function. Note that if a coloring with weight k is fixed by a permutation g, then the elements in the same cycle of g are assigned by the same color (so have the same weight) in the coloring. So a cycle length of j contribute totally weight of $j \times w$ to the coloring and has l_w choices to assign, if its elements are assigned by a color of weight w. What is more, the sum of the weights of all cycles of g equals to k. Thus,

$$\Psi_k(g) = \sum_{\sum_{j=1}^{m} \sum_{i=1}^{b_j} j \times w_{j,i} = k} \prod_{j=1,\ldots,m} \prod_{i=1,\ldots,b_j} l_{w_{j,i}},$$

which equals to the coefficient of x^k in the polynomial

$$L(x)^{b_1} L(x^2)^{b_2} \cdots L(x^m)^{b_m}.$$

Thus, we have

$$Z(x) = \frac{1}{|G|} \sum_{g \in G} L(x)^{b_1} L(x^2)^{b_2} \cdots L(x^m)^{b_m}, \tag{2}$$

which nicely corresponds to the cycle index of G.

2.2 Recursion counting formula for the numbers of *CI*-different and *CC*-different MTL-polyinositols

We can suppose the planted hexagonal ring of each MTL-polyinositol is fixed on the average plane such that the planted bond is above the average plane. It would be helpful to consider a MTL-polyinositol with n hexagonal rings as one constructed by fusing a C–OH bond of a ‘smaller’ TL-polyinositol or an -OH ligand to each of the five numbered O–H bonds of the planted inositol rings, such that the total number of all the hexagonal rings is equal to n. We call these smaller TL-polyinositols the branches of the planted ring. Since each branch has a specified C–OH bond to be fused to the planted ring, we may treat this branch as a MTL-polyinositol with the fused C–OH bond as its planted bond.

We denote by $(T_1, T_2, \ldots, T_5)$ the MTL-polyinositol with T_i ($i \in \{1, 2, \ldots, 5\}$) as the i-th branch (some braches may be an -OH ligand) of its planted ring, see Fig. 1h.

Note that each branch can be treated as a color with the number of hexagonal rings it contains as its weight. Then each MTL-polyinositol with n rings can be treated as a coloring of the planted ring with weight $n-1$ which is defined as follows: the i-th of its five positions (each of which may above or below the average plane) is assigned with color T_i, for $i = 1, 2, \ldots, 5$, and the sum of the weights of the colors equals to $n-1$. Then the number of MTL-polyinositol with n rings equals to the number of the nonequivalent colorings with wight $n-1$ using the color in C under G, where C is the set of *CI*-different MTL-polyinositols and G is the group by which $(T_1, T_2, T_3, T_4, T_5)$ is interconverted.

In the case when charity is ignored, G is the identity group, i.e., $G = G_1 = \{e\} = \{(1)(2)(3)(4)(5)\}$. Because the planted bond and planted ring have been fixed. $(T_1, T_2, T_3, T_4, T_5)$ can not be interconverted by any other permutation. Using the same notations to that defined in Sect. 2.1, we have $r_n = z_{n-1}$, $l_n = r_n$, for $n = 1, 2, \ldots$. And let $l_0 = r_0 = 1$. Because when we color the root ring, -OH is a color choice. Then $R(x) = 1 + xZ(x)$. Suppose a coloring $\mathscr{C}$ is left fixed by permutation g. Then for $\mathscr{C}$, each cycle of g has $2l_i = 2r_i$ choices to assign now, if the color weight of each element in the cycle is i, since either the side above or below of each of the five positions can be assigned. So by a similar discussion to that before (2), and through the cycle index of G_1, we can deduce that

$$Z(x) = (2R(x))^5,$$

here.

Theorem 1 *The generating function* $R(x)$ *satisfies*

$$R(x) = 1 + 32xR^5(x) = 1 + \sum_{n=1}^{\infty} \frac{32^n}{n} \binom{5n}{n-1} x^n. \tag{3}$$

Proof By the discussion above, we have the left equation of (3) holds.

On the other hand, let $y = 32x$, *i.e.*, $x = \frac{y}{32}$. Let $Q(y) = R(\frac{y}{32}) = R(x)$. Then

$$Q(y) = R\left(\frac{y}{32}\right) = 1 + 32 \times \frac{y}{32} R^5\left(\frac{y}{32}\right) = 1 + yQ^5(y).$$

It is known ([43], Problem III, 209, pp. 146, 348) that the solution of the equation for $Q(y)$ above is

$$Q(y) = 1 + \sum_{n=1}^{\infty} \frac{1}{n} \binom{5n}{n-1} y^n,$$

which implies that

$$R(x) = 1 + \sum_{n=1}^{\infty} \frac{32^n}{n} \binom{5n}{n-1} x^n.$$

□

In the case when charity is considered, we suppose the mirror face is vertical to the average plane and parallel to the planted rigid bond. Then after reflection, the planted ring of every MTL-polyinositol is still on the average plane and the planted bond is still above the average plane. Then the group by which $(T_1, T_2, T_3, T_4, T_5)$ is interconverted is $G_2 = \{e, \alpha\}$, where $\alpha = (\overline{15})(\overline{24})(\overline{3})$ is the reflection permutation. An overlined cycle $(\overline{\cdots ij \cdots})$ suggests that the color T_i in ith position is permutated to jth position and is reflected to $\overline{T}_i$, where $\overline{T}_i$ is enantiomeric to T_i. The cycle index of G_2 is

$$\frac{1}{2}\left(x_1^5 + \overline{x}_1\overline{x}_2^2\right),$$

Using the same notations to that defined in Sect. 2.1, now we have $\overline{r}_n = z_{n-1}$, for $n = 1, 2, \ldots$. And $l_n = r_n$, for $n = 0, 1, 2, \ldots$. Then $\overline{R}(x) = 1 + xZ(x)$. Note that if a coloring is left fixed by a permutation g, then an overlined odd cycle must be assigned by achiral colors (so has $2b_i$ choices to assign), while any other cycle has $2b_j$, if i and j the color weights of the elements in the corresponding cycle, respectively. So by a similar discussion to that before Theorem 1, and the cycle index of G_2 we can deduce that

$$Z(x) = \frac{1}{2}x\left[(2R(x))^5 + (2B(x))(2R(x^2))^2\right]$$

here.

Theorem 2 *The generating function $\overline{R}(x)$ satisfies*

$$\overline{R}(x) = 1 + \frac{1}{2}x\left[32R^5(x) + 8R^2(x^2)B(x)\right]. \tag{4}$$

Proof By the discussion above and simply (4) holds. □

Note 2. by Note 1, we have

$$B(x) = 2\overline{R}(x) - R(x). \tag{5}$$

Thus, (3), (4) and (5) provide a recursion algorithm which can be worked by, e.g., Maple Soft Program, for counting r_n, b_n and $\overline{r}_n$.

2.3 Recursion counting formula for *CI*-different tree-like polyinositols

In graph theory, Dissimilarity Characteristic Theorem [18,26] for trees establishes a connection between the generating functions for trees and planted trees. This connection has been extensively used for various species of trees. In the following we will specify the Dissimilarity Characteristic Theorem in accord with tree-like polyinositols, when charity is ignored.

When we delete all leaf vertices and short edges in a contracted tree T, and change each long edge to a line, we will get a unique tree in graph theory. We call it the *topological tree* of T. It is known that the set of trees with n vertices can be partitioned into two classes, i.e., central trees and bicentral trees [44]. A center tree contains a vertex (called the central vertex) whose deletion will decompose the tree into components each of which contains less than $\frac{n}{2}$ vertices, while a bicentral tree contains an edge (called the central edge) whose deletion will decompose the tree into two components both containing $\frac{n}{2}$ vertices. We call a contracted tree *central* (or *bicentral*) if its topological tree is central (or bicentral). A *central vertex* and a *central long edge* in a contracted tree can be defined correspondingly.

Let T be a contracted tree. A *CI-automorphism* of T is a rotation of T, after which, the space which T occupies coincides to that it occupied before. Note that a CI-automorphism should rotate an inner (leaf) vertex to an inner (leaf) vertex, and a long (short) edge to a long (short) edge. Two inner vertices or two long edges in T are called *CI-similar* to each other if there is an CI-automorphism of T which transfers one to the other, and are called *CI-dissimilar* to each other otherwise. A long edge e is called *CI-symmetric* if there is a nontrivial CI-automorphism which transfers e to itself, and is called *CI-asymmetric* otherwise. We denote by $v(T)$, $e(T)$ and $s(T)$ the numbers of CI-dissimilar inner vertices, CI-dissimilar CI-asymmetric long edges and CI-symmetric long edges, respectively.

Theorem 3 (CI-Dissimilarity Characteristic Theorem) *In any contracted tree T, we have*

$$v(T) - e(T) = 1. \tag{6}$$

Proof For a central contracted tree, let v be the central vertex. For each long edge e, denote by u_e be the incident inner vertex of e which is further from v. Then each long edge e has a unique u_e. For each inner vertex u other than v, there is a unique long edge e such that $u = u_e$. Note that any CI-automorphism will transfer v to itself, for the uniqueness of central vertex. Then two long edges e_1 and e_2 are CI-similar if and only if u_{e_1} and u_{e_2} are CI-similar. Thus there is a one to one correspondence between CI-similar classes of long edges and CI-similar classes of inner vertices, except one CI-similar class $\{v\}$. Thus (6) holds for central contracted trees.

For a bicentral contracted tree, let e be the central edge. For each inner vertex v, denote by f_v be the incident long edge of v which is nearer from e. Then each inner vertex v has a unique f_v. For each long edge f other than e, there is a unique inner vertex v such that $f = f_v$. And there are two inner vertex v_1 and v_2 such that $e = f_{v_1} = f_{v_2}$. Note that any CI-automorphism will transfer e to itself, for the uniqueness of central edge. Then two inner vertices u and v are CI-similar if and only if f_u and f_v are CI-similar. If the central edge is CI-symmetric, there is a one to one correspondence between CI-similar classes of inner vertices and CI-similar classes of long edges. So $v(T) - e(T) = 1$, as $\{e\}$ is one CI-similar class. If the central edge is not CI-symmetric, then each inner vertex and each long edge is a CI-similar class, respectively. So $v(T) - e(T) = 1$ also holds. This completes our proof. □

Let $\mathcal{T}_n^{CI}$ be the set of all CI-different contracted trees with n ($n \geq 1$) inner vertices. Let

$$v_n = \sum_{T\in \mathcal{T}_n^{CI}} v(T), \;\; e_n = \sum_{T\in \mathcal{T}_n^{CI}} e(T) \;\text{ and }\; s_n = \sum_{T\in \mathcal{T}_n^{CI}} s(T). \tag{7}$$

Combining (7) with (6), we get that

$$v_n - e_n = |\mathcal{T}_n^{CI}| = t_n. \tag{8}$$

Note that $s_n = 0$, if n is odd; and $s_n = r_{\frac{n}{2}}$ if n is even, by definition. Let

$$V(x) = \sum_{n=1}^{\infty} v_n x^n, \;\; E(x) = \sum_{n=1}^{\infty} e_n x^n \;\text{ and }\; S(x) = \sum_{n=1}^{\infty} s_n x^n,$$

be the generating functions of v_n, e_n and s_n, respectively. Then

$$T(x) = V(x) - E(x) \;\text{ and }\; S(x) = R(x^2) - 1. \tag{9}$$

We discuss the expressions of $V(x)$ and $E(x)$ next.

For an inner vertex x and a long edge e in a contracted tree T, we denote by T_x and T_e the inner vertex rooted tree and the long edge rooted tree obtained from T by making x and e as their roots, respectively. Note that x have six branches, some of which may be a single leaf vertex, while e have two branches each of which contains at least one inner vertex. Let x_1 and x_2 are any two inner vertices a contracted tree T which are *CI*-dissimilar to each other. Then T_{x_1} and T_{x_2} are *CI*-different. Furthermore, any two inner vertex rooted trees obtained from two *CI*-different contracted trees are *CI*-different. This implies that the number of *CI*-different inner vertex rooted trees of order n equals to v_n. Similarly, the number of *CI*-different long edge rooted trees of order n equals to $e_n + s_n$.

We now calculate v_n and $e_n + s_n$ by enumerating *CI*-different ring rooted TL-polyinoisitols and C–O–C bond rooted TL-polyinoisitols as they are equivalent. As before, we treat a ring rooted TL-polyinoisitol as a coloring of the the rooted ring by its six branches T_1, T_2, T_3, T_4, T_5 and T_6. Then the number of *CI*-different ring rooted TL-polyinositols with n hexagonal rings, equals to the number of nonequivalent colorings of the rooted ring under G_6 with weights $n-1$, where G_6 is the group by which $(T_1, T_2, T_3, T_4, T_5\, T_6)$ is *CI*-interconverted, see Fig. 2a and b. Note that $G_6 = D_6 = \{e, \beta, \gamma, \gamma^2, \gamma^3, \gamma^4, \gamma^5, \beta\gamma, \beta\gamma^2, \beta\gamma^3, \beta\gamma^4, \beta\gamma^5\}$, where $\beta = (\widetilde{16})(\widetilde{25})(\widetilde{34})$ is derived from a vertical rotation which changes the two sides of the rooted ring face, and $\gamma = (123456)$ is derived from a horizontal rotation which doesn't. A tilded cycle $(\widetilde{\cdots ij \cdots})$ represents that, the branch in the i-th position is rotated to the j-position on the other side of the average plane. We write the cycle index of D_6 as

$$\frac{1}{12}\left(x_1^6 + x_2^3 + 2x_3^2 + 2x_6 + 3\tilde{x}_1^2\tilde{x}_2^2 + 3\tilde{x}_2^3\right),$$

where tilded variants represent tilded cycles.

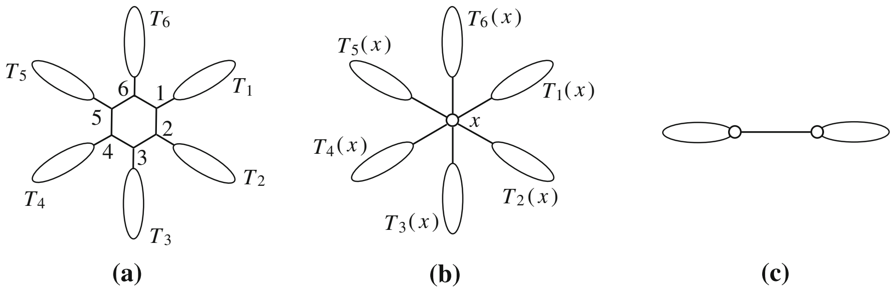

Fig. 2 **a** A hexagonal ring and its six branches in a tree-like polyinositol. **b** The corresponding vertex and six branches in the contracted tree. **c** A long edge and its two branches

Using the same notion to that in Sect. 2.1, now we have $v_n = z_{n-1}$, for $n = 1, 2, \ldots$. And $l_n = r_n$, for $n = 0, 1, 2, \ldots$. Then $T(x) = xZ(x)$. Note that a permutation g contains a tilded odd cycle, then no coloring can be left fixed by g. And every cycle of a permutation without any tilded odd cycle have $2r_i$ color choices to assign, where i is the weight of each element in the cycle. By a similar discussion to that before Theorem 1 and 2, and the cycle index of D_6, we have

$$Z(x) = \frac{1}{12}\left[(2R(x))^6 + 4\left(2R\left(x^2\right)\right)^3 + 2\left(2R\left(x^3\right)\right)^2 + 2\left(2R\left(x^6\right)\right)\right],$$

here. And so

$$V(x) = \frac{x}{12}\left[(2R(x))^6 + 4\left(2R\left(x^2\right)\right)^3 + 2\left(2R\left(x^3\right)\right)^2 + 2\left(2R\left(x^6\right)\right)\right]. \quad (10)$$

Similarly, the number of CI-different long edge rooted TL-polyinositols equals to the number of nonequivalent colorings of the rooted C–O–C bond edge under S2, see Fig. 2c, where $S_2 = \{(1)(2), (12)\}$, whose cycle index is

$$\frac{1}{2}\left(x_1^2 + x_2\right).$$

Using the same notion to that in Sect. 2.1, now we have $e_n + s_n = z_n$, for $n = 2, 3, \ldots$ (note that $e_1 = s_1 = 1$). And $l_n = r_n$, for $n = 1, 2, \ldots$. Then $E(x) + S(x) = Z(x)$. By calculating and a similar discussion to that before Theorem 1, we deduce

$$E(x) + S(x) = Z(x) = \frac{1}{2}\left[(R(x) - 1)^2 + \left(R\left(x^2\right) - 1\right)\right], \quad (11)$$

here.

Theorem 4 *The generating function $T(x)$ of the number of TL-polyinositols ignoring chirality satisfies*

$$T(x) = \frac{x}{3}\left[16R^6(x) + 8R^3\left(x^2\right) + 2R^2\left(x^3\right) + R\left(x^6\right)\right] \\ -\frac{1}{2}\left[(R(x)-1)^2 - \left(R\left(x^2\right)-1\right)\right], \tag{12}$$

Proof By (9)–(11), we have (12) holds. □

Note 3. By (12), we can count t_n through the numbers $r_0, r_1, \ldots, r_n$ with the help of a simple algorithm worked by Maple Soft Program.

2.4 Recursion counting formula for *CC*-different tree-like polyinositols

A *CC-automorphism automorphism* of a contracted tree T is a rotation or a product of a rotation and reflection of T, after which, the space which T occupies coincides to that it occupied before. Two inner vertices or two long edges in T are called *CC-similar* to each other if there is an *CC*-automorphism of T which transfers one to the other, and are called *CC-dissimilar* to each other otherwise. A long edge e is called *CC-symmetric* if there is a nontrivial *CC*-automorphism which transfers e to itself, and is called *CC-asymmetric* otherwise. Note that an long edge is *CC*-symmetric if and only if its two branches are identical or a pair of enantiomers. We denote by $\overline{v}(T)$, $\overline{e}(T)$ and $\overline{s}(T)$ the number of *CC*-dissimilar inner vertices, *CC*-dissimilar *CC*-asymmetric long edges, and *CC*-symmetric long edges, respectively.

Theorem 5 (CC-Dissimilarity Characteristic Theorem) *In any contracted tree T we have*

$$\overline{v}(T) - \overline{e}(T) = 1. \tag{13}$$

Proof The proof is analogous to that in Theorem 3. □

Let $\overline{\mathcal{T}}_n^{CC}$ be the set of all *CC*-different contracted trees. Let

$$\overline{v}_n = \sum_{T\in \mathcal{T}_n^{CC}} \overline{v}(T), \quad \overline{e}_n = \sum_{T\in \mathcal{T}_n^{CC}} \overline{e}(T) \text{ and } \overline{s}_n = \sum_{T\in \mathcal{T}_n^{CC}} \overline{s}(T). \tag{14}$$

Combining (14) with (13), we get that

$$\overline{v}_n - \overline{e}_n = |\overline{\mathcal{T}}_n^{CC}| = \overline{t}_n. \tag{15}$$

Note that $\overline{s}_n = 0$, if n is odd; and $\overline{s}_n = \overline{r}_{\frac{n}{2}} + (r_{\frac{n}{2}} - \overline{r}_{\frac{n}{2}}) = r_{\frac{n}{2}}$ if n is even, by definition. In fact, $\overline{r}_{\frac{n}{2}}$ is the number when the two branches are identical, while $(r_{\frac{n}{2}} - \overline{r}_{\frac{n}{2}})$ is the number when the two branches are a pair of enantiomers which are not identical. Let

$$\overline{V}(x) = \sum_{n=1}^{\infty} \overline{v}_n x^n, \quad \overline{E}(x) = \sum_{n=1}^{\infty} \overline{e}_n x^n \text{ and } \overline{S}(x) = \sum_{n=1}^{\infty} \overline{s}_n x^n,$$

be the generating functions of $\overline{v}_n$, $\overline{e}_n$ and $\overline{s}_n$, respectively. Then

$$\overline{T}(x) = \overline{V}(x) - \overline{E}(x) \text{ and } \overline{S}(x) = R(x^2) - 1. \tag{16}$$

By an analogous discussion to that in the previous subsection, we can obtain that $\overline{v}_n$ and $\overline{e}_n + \overline{s}_n$ are exactly the numbers of CC-different inner vertex rooted trees and long edge rooted trees of order n, respectively. And they equal to the numbers of nonequivalent colorings to the rooted ring and rooted C–O–C bond by branches under $\overline{D}_6$ and $\overline{S}_2$, whose cycle indices are

$$\begin{aligned}&\frac{1}{24}\left[\left(x_1^6 + x_2^3 + 2x_3^2 + 2x_6 + 3\widetilde{x}_1^2\widetilde{x}_2^2 + 3\widetilde{x}_2^3\right)\right.\\&\left.\quad + \left(\overline{\widetilde{x}}_1^6 + \overline{\widetilde{x}}_2^3 + 2\overline{\widetilde{x}}_3^2 + 2\overline{\widetilde{x}}_6 + 3\overline{x}_1^2\overline{x}_2^2 + 3\overline{x}_2^3\right)\right],\end{aligned}$$

and

$$\frac{1}{4}\left[\left(x_1^2 + x_2\right) + \left(\overline{x}_1^2 + \overline{x}_2\right)\right],$$

respectively. By calculating and a similar discussion to that in the previous subsection, we have

$$\begin{aligned}\overline{V}(x) = \frac{x}{24}&\left[(2R(x))^6 + 4\left(2R\left(x^2\right)\right)^3 + 2\left(2R\left(x^3\right)\right)^2 + 2\left(2R\left(x^6\right)\right)\right.\\&\left.+\left(2R\left(x^2\right)\right)^3 + 2\left(2R\left(x^6\right)\right) + 3(2B(x))^2\left(2R\left(x^2\right)\right)^2 + 3\left(2R\left(x^2\right)\right)^3\right],\end{aligned}$$

and

$$\overline{E}(x) + \overline{S}(x) = \frac{1}{4}\left[(R(x)-1)^2 + \left(R\left(x^2\right) - 1\right) + (B(x) - 1)^2 + \left(R\left(x^2\right) - 1\right)\right].$$

Theorem 6 *The generating function $\overline{T}(x)$ satisfies*

$$\begin{aligned}\overline{T}(x) = &\frac{x}{3}\left[8R^6(x) + 8R^3\left(x^2\right) + R^2\left(x^3\right) + R\left(x^6\right)\right]\\&-\frac{1}{4}R^2(x) + \frac{1}{2}R(x) + \frac{1}{2}R\left(x^2\right) + \frac{1}{4}B(x) - 1,\end{aligned} \tag{17}$$

Proof By (16) and the expressions of $\overline{V}(x)$ and $\overline{E}(x)$, (17) holds. □

Note 4. By (17), we can count $\overline{t}_n$ through the numbers $r_0, \ldots, r_n$ and $b_0, \ldots, b_n$ with the help of Maple Soft Program.

2.5 Asymptotic analysis

In this section, we give an asymptotic analysis for the numbers $r_n,\ t_n,\ \overline{r}_n$ and $\overline{t}_n$, by applying the 'twenty-step algorithm' summarized by Harary et al [19]. We denote by $r(n),\ t(n),\ \overline{r}(n)$ and $\overline{t}(n)$ the asymptotic values of $r_n,\ t_n,\ \overline{r}_n$ and $\overline{t}_n$, respectively. The relations (3), (4), (12) and (17) obtained in the previous sections are the bases for implementing the twenty steps. The key points are as follows:

(1). Show that $\sigma = 0.00256$, where σ is the radius of convergence of $R(x)$.
(2). From (3) we define a function $F(x, y) = 32xy^5 - y + 1$ and prove that $F(x, y)$ is analytic for all y and x with $|x| < \sigma^{\frac{1}{2}}$. Moreover, $F(x, R(x)) = 0$ for all x with $|x| \le \sigma$.
(3). Show that $F_y(x, R(x)) = 0$ and, consequently, $160R^5(\sigma) = 1$, combining which to $F(\sigma, R(\sigma)) = 0$ we can compute $R(\sigma) = 1.25$.
(4). Show that σ is the unique singularity of $R(x)$ on the circle of convergence [45] and a branch point of order 2 for $R(x)$, from which we can rewrite $R(x)$ as the form

$$R(x) = R(\sigma) - k_1(\sigma - x)^{\frac{1}{2}} + k_2(\sigma - x) + k_3(\sigma - x)^{\frac{3}{2}} + \cdots . \tag{18}$$

(5). From (3) and (18), the coefficient k_1 can be expressed in terms of σ and $R(\sigma)$, which gives that

$$k_1 = \frac{5^3}{4^2} = 7.8125.$$

(6). Applying a result of Polya (lemma on page 84 of [2]), we finally get the asymptotic value of r_n:

$$r_n \sim r(n) = \frac{k_1}{2}\left(\frac{\sigma}{\pi}\right)^{\frac{1}{2}} n^{-\frac{3}{2}}\sigma^{-n}, \quad \text{as} \quad n \to \infty.$$

The discussions for $t_n,\ \overline{r}_n$ and $\overline{t}_n$ are analogous which give that

$$t_n \sim t(n) = \frac{3l_3}{4}\left(\frac{\sigma^3}{\pi}\right)^{\frac{1}{2}} n^{-\frac{5}{2}}\sigma^{-n}, \quad \text{as} \quad n \to \infty,$$

$$\overline{r}_n \sim \overline{r}(n) = \frac{q_1}{2}\left(\frac{\sigma}{\pi}\right)^{\frac{1}{2}} n^{-\frac{3}{2}}\sigma^{-n}, \quad \text{as} \quad n \to \infty,$$

and

$$\overline{t}_n \sim \overline{t}(n) = \frac{3p_3}{4}\left(\frac{\sigma^3}{\pi}\right)^{\frac{1}{2}} n^{-\frac{5}{2}}\sigma^{-n}, \quad \text{as} \quad n \to \infty,$$

where

$$
\begin{aligned}
\frac{3}{4}l_3 &= \frac{k_1}{2}\left(\frac{R(\sigma)-1}{\sigma}\right) = \frac{5^8}{4^5} = 381.4697265625,\\
q_1 &= \frac{k_1}{2} = \frac{5^3}{2\times 4^2} = 3.90625
\end{aligned}
$$

and

$$
\frac{3}{4}p_3 = \frac{k_1}{4}\left(\frac{R(\sigma)-1}{\sigma}\right) = \frac{5^8}{2\times 4^5} = 190.73486328125.
$$

The detailed process of the above arguments is included in the supplementary material.

Note 5. We can see that $r(n) = 2\overline{r}(n)$ and $t(n) = 2\overline{t}(n)$ which imply that almost all MTL-polyinositols and TL-polyinositols are chiral (Tables 1, 2).

2.6 Numerical results

In Table 1 and Table 2 we list the numerical results for the numbers r_n and $\overline{r}_n$, t_n and $\overline{t}_n$, respectively, for n from 1 up to 16. The number of MTL-polyinositols and

Table 1 The numerical results for the numbers r_n and $\overline{r}_n$ for the number n of hexagonal rings from 1 to 16

n	r_n	$\overline{r}_n$
0	1	1
1	32	20
2	5120	2592
3	1146880	573952
4	298844160	149428224
5	84892712960	42446467072
6	25502442061824	12751222538240
7	7967336132771840	3983668094959616
8	2562351375392440320	1281175688111456256
9	842678201979617935360	421339100997916557312
10	282086756943037076602880	141043378471641045532672
11	95799423035664196530339840	47899711517834536732852224
12	32925528674152582159427174400	16462764337076328909785530368
13	11430767567997743931496668856320	5715383783998872729037037371392
14	4002697650510768892543602125701120	2001348825255384458341277639901184
15	1412072851444666880340899212075991040	706036425722333440416447740566831104
16	501392147316191287339969610550251356160	250696073658095643673931264768516030464

Table 2 The numerical results for the numbers t_n and $\bar{t}_n$ for the number n of hexagonal rings from 1 to 16

n	t_n	$\bar{t}_n$
1	9	8
2	528	288
3	82176	41472
4	16605056	8306880
5	3858808832	1929484288
6	980863729664	490432905216
7	265577882983776	132788961720672
8	75363275896258560	37681638230458368
9	22175742160587980800	11087871085962592256
10	6716351355829045166080	3358175677996999376896
11	2082596152950163872153600	1041298076476772274143232
12	658510573483064394409574400	329255286741557487851274240
13	211680880888847398144107174912	105840440444424224866960759808
14	69012028457082226268902585794560	34506014228541121161023614615552
15	22775368571688175580659593561243648	11387684285844087958973989760532480
16	7596850716911989203401927496470364160	3798425358455994604314781338778468352

TL-polyinositols with n hexagonal rings for n from 17 up to 50 are tabulated in the supplementary material.

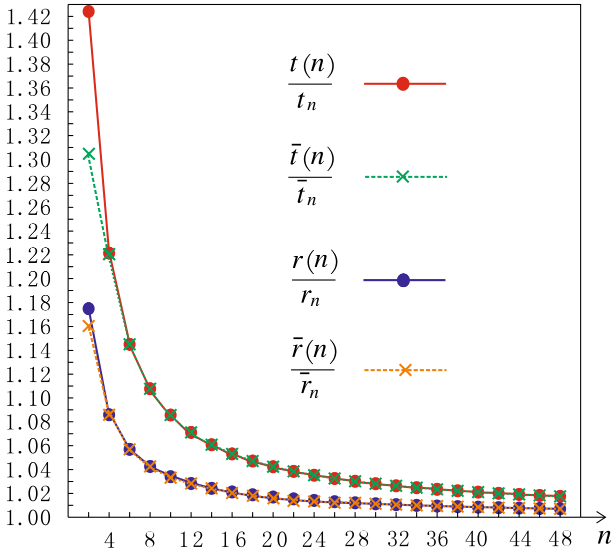

Fig. 3 The horizontal axis represents the number of inositol rings and the vertical axis represents the ratios between the asymptotic values and the numerical results for MTL-polyinositols and TL-polyinositols

For better understanding their asymptotic behaviors, in Fig. 3 we also illustrate the ratios $r(n)/r_n$, $\bar{r}(n)/\bar{r}_n$, $t(n)/t_n$ and $\bar{t}(n)/\bar{t}_n$ for n up to 48. Figure 3 shows that the asymptotic values are well-fitting to the numerical results.

3 Supplementary material

The detailed procedures of the asymptotic analysis and the numbers of MTL-polyinositols and TL-polyinositols with n hexagonal rings for n from 17 up to 50 are included in the supplementary material.

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