

# Symmetry property of dendrimers

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A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. In this paper, the mathematical tools of group theory have been used extensively for the analysis of the symmetry properties of a new class of these macromolecules.

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## 1. Introduction

Dendrimers are one of the main objects of nanobiotechnology. They are large molecules and offer a challenge to theoretical chemistry. Their step-wise growth follows a mathematical progression. In an exact phrase, dendrimers are hyperbranched macromolecules, showing a rigorous, aesthetically appealing architecture [1-3].

A molecule  $M$  is a complex entity which has extension in the 3D space. This feature is implicit in stereochemical models. Some information of  $M$  is lost when it is depicted in a 2D framework. However, the 2D description encodes all the connectivity properties of  $M$ . This 2D framework is usually called the molecular graph of  $M$ .

We first recall some algebraic definitions that will be used in the paper. The symmetry of a physical object can be formalized by the notion of a group action: every element of the group "acts" like a bijective map on some set. Here, by symmetry of a molecule, we mean the automorphism group symmetry of its molecular graph. This type of symmetry also called a topological symmetry, accounts only for the bond relations between atoms, and does not fully determine molecular geometry [4]. To clarify this notion, we assume that  $G$  is a group and  $X$  is a set.  $G$  is said to act on  $X$  when there is a map  $\phi : G \times X \rightarrow X$  such that for all elements  $x \in X$ , (i)  $\phi(e, x) = x$  where  $e$  is the identity element of  $G$ , and, (ii)  $\phi(g, \phi(h, x)) = \phi(gh, x)$  for all  $g, h \in G$ . In this case,  $G$  is called a transformation group;  $X$  is called a  $G$ -set, and  $\phi$  is called the group action. For simplicity we define  $gx = \phi(g, x)$ . In a group action, a group permutes the elements of  $X$ . The identity does nothing, while a composition of actions corresponds to the action of the composition. For a given  $X$ , the set  $\{gx \mid g \in G\}$ , where the group action moves  $x$ , is called the group orbit of  $x$ . The subgroup which fixes is the isotropy group of  $x$ .

Let  $G$  be a group and  $N$  be a subgroup of  $G$ .  $N$  is called a *normal subgroup* of  $G$ , if for any  $g \in G$  and  $x \in N$ ,  $g^{-1}xg \in N$ . Moreover, if  $H$  is another subgroup of  $G$  such that  $H \cap N = \{e\}$  and  $G = HN = \{xy \mid x \in H, y \in N\}$ , then we say that  $G$  is a semidirect product of  $H$  by  $N$  denoted by  $H$

:  $N$ . Suppose  $X$  is a set. The set of all permutations on  $X$ , denoted by  $S_X$ , is a group which is called the symmetric group on  $X$ . In the case that,  $X = \{1, 2, \dots, n\}$ , we denote  $S_X$  by  $S_n$  or  $\text{Sym}(n)$ .

Let  $H$  be a permutation group on  $X$ , a subgroup of  $S_X$ , and let  $G$  be a group. The set of all mappings  $X \rightarrow G$  is denoted by  $G^X$ , i.e.  $G^X = \{f \mid f: X \rightarrow G\}$ . It is clear that  $|G^X| = |G|^{|X|}$ . We put  $G \wr H = G^X \times H = \{(f, \pi) \mid f \in G^X, \pi \in H\}$ . For  $f \in G^X$  and  $\pi \in H$ , we define  $f_\pi \in G^X$  by  $f_\pi = f \circ \pi^{-1}$ , where " $\circ$ " denotes the composition of functions. It is easy to check that the composition law  $(f; \pi)(f'; \pi') = (ff'_\pi; \pi \pi')$ , makes  $G \wr H$  into a group. This group is called the wreath product of  $G$  by  $H$  [5].

In some leading papers, Balasubramanian [6–13] introduced the wreath product formalism for computing symmetry of molecules. Then the present authors in some research papers continued the mentioned works of Balasubramanian [14-40] to present a computational approach which is valuable in practical problems. We encourage the readers to consult also papers [41-43] for background materials as well as basic computational techniques. Our calculation given the paper was done by the computer algebra system GAP [44], which is freely accessible from internet.

## 2. Main results and discussion

In this section, we describe our computational approach by GAP in computing symmetry of dendrimer, Fig. 1. This method is appropriate for molecules which consist of a number of  $XY_2$  or  $XY_3$  groups (as  $CH_3$  or  $NO_2$ ) attached to a rigid framework. An example of such molecule is a dendrimer  $D[n]$ , which is considered here in some detail, see Fig. 1. We first compute the number of vertices of  $D[n]$ . Using a simple counting argument, one can see that

$$|V(D[n])| = 4 + 4 \times 3 + 4 \times 3^2 + \dots + 4 \times 3^{n-1} = 4 \times \frac{3^n - 1}{3 - 1} = 2 \times (3^n - 1).$$

With a geometric consideration of dynamic symmetries of the molecules we will show that the symmetry group of the molecule can be specified by wreath product of some known groups. Then based on the structure of the group we apply GAP as a useful package for computing the generating set and also the group structure of this molecule.

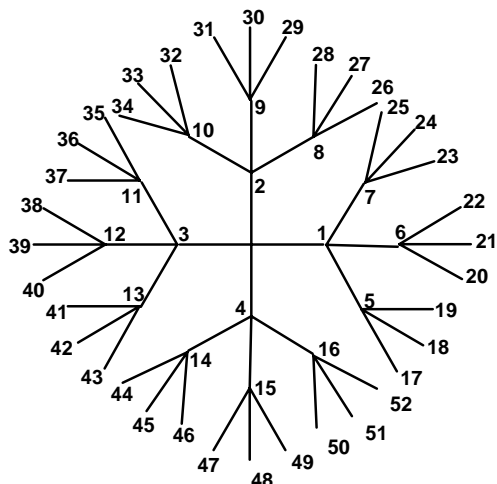


Fig. 1. The third generation of dendrimer molecule  $D[n]$ .

We consider the dendrimer molecule  $D[n]$ , Fig. 1. In order to characterize the symmetry of this molecule we note that each dynamic symmetry operation of  $D[1]$ , considering the rotations of  $XY_3$  groups in different generations of the whole molecule  $D[n]$ , is composed of  $n$  sequential physical operations. We first have a physical symmetry of the framework (as we have to map the  $XY_3$  groups on  $XY_3$  groups which are on vertices of the framework). Such operations form the group  $G$  of order 6, which as is well known to be isomorphic to  $S_3$  or  $Sym(3)$ . After accomplishing the first framework symmetry operation we have to map each of the three  $XY_3$  group on itself in the first generation and so on. Therefore, the symmetry group of dendrimer  $D[n]$  is isomorphic to  $(S_3 \sim (S_3 \sim S_3) \sim \dots \sim (S_3 \sim S_4) \dots)$ . To compute the order of this group, we assume that  $a_0 = 4!$ . Then the order of the symmetry of  $D[n]$  can be computed from the following recursive formula:

$$a_n = 6^{4 \times 3^{n-1}} a_{n-1} \quad n \geq 1.$$

We now compute a generating set for this group. To do this, we define permutations  $b_i$  and  $c_i$ ,  $1 \leq i \leq 2 \times 3^n - 1$ , as follows:

$$b_i = (2+3i, 3+3i) ; \quad c_i = (2+3i, 3+3i, 4+3i) \quad 1 \leq i \leq 2 \times 3^n - 1.$$

All calculations given here are checked by computer algebra system GAP. Our programs are accessible from authors upon request.

### 3. Conclusions

In this paper a general method for computing symmetry of a dendrimer is presented, which is useful for hyperbranched compounds. We proved that the symmetry groups of these molecules can be reformulated as wreath product of a sequence of well-known finite groups. Using computer algebra system GAP generating sets for these classes of dendrimers are computed. Our method is general and can be applied to other dendrimers.

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