Proceedings of the International Conference on Nanotechnology: Fundamentals and Applications
Ottawa, Ontario, Canada, 4-6 August 2010
Paper No. 472

Automorphism group of a Family of Dendrimer Nanostars

E. Zahedi, M.H.Khalifeh and H. Faramarzi
School of mathematics, college of science,
University of Tehran, Tehran, Iran.
E.zahedi@ut.ac.ir, khalife@khayam.ut.ac.ir, faramarzi@khayam.ut.ac.ir

A.R.Ashrafi
Institue of nanoscience and nanotechnology, university of kashan
Alir.ashrafi@gmail.com

ABSTRACT

A dendrimer nanostar 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 automorphism group of the molecular graph of these nanomolecules. We prove a theorem that can be used as a tool for recognition of these types of molecular graphs automorphism groups. And as an example we compute the automorphism group of a dendrimer nanostar.

1 INTRODUCTION

Dendrimers are on of the main objects of nanobiotechnology. They possess a well defined molecular topology. Their step-wise growth follows a mathematical progression.

In an exact phrase, dendrimers are hyperbranched macromolecules, showing a rigorous, aesthetically appealing architecture [1-3]. Group theory is one of the most important branches of mathematics for studying molecular structures of compounds. By using tools taken from the group theory and graph theory, it is possible to evaluate chemical structures according to their symmetry.

Let G be a graph, V (G) and E (G) show the set of its vertices and its edges respectively. Here, we mean the automorphism group symmetry of its molecular graph, by symmetry of a molecule and some algebraic definition that will be used in paper and for the more information you can consider [6-17].

Two graphs are isomorph if there is a bijective between their vertex set and their edge set such that preserve adjacency. Consider a permutation of (G) such that preserve isomorphism all such permutations constitute a group we say automorphism group of the graph G and show with Aut(G).

The symmetry of a physical object can be formalized by the action notion: every element of the group "acts" like a bijective map on some set. To clarify this notion, we assume that G is a group and Ω is a set. G is said to act on Ω ($G|_{\Omega}$),when there is a map $\rho: G \times \Omega \rightarrow \Omega$ such that $\rho(g, \omega) = \omega^{g}$and for all elements $\omega \in \Omega$, $\omega^{e} = \omega$ where e is the identity element of G, and $(\omega^{g})^{h}=\omega^{gh}$ for all $g, h \in G$. In this case, G is called a transformation group, *Ω* is called a G-set, and ρ is called a group action. For a given *Ω*, the set; $\omega^{G}= \{\omega^{g} \mid g \in G\}$, where the group action moves ω, is called a group orbit of ω. Indeed for a graph G, Aut(G) acts on V(G).

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 $H \rtimes N$.

Suppose Ω is a set. The set of all permutations on *Ω*, denoted by S_{Ω}, S_{Ω} is a group which is called the symmetric group on *Ω*. In the case $\Omega = \{1,2,3,..,n\}$, we denote S_{Ω} by S_n. Let $\Omega=\{1,2,3,..,n\}$ and H

be a arbitrary group, and $\mathrm{Funk}(\Omega, H)$ be the set of all functions from Ω to H it is easy to check that $\mathrm{Funk}(\Omega, H) \rtimes S_n = H \wr S_n$ be a group with composition law

$$(f_1, \pi_1).(f_2, \pi_2) = \{ (f_1 f_2^{\pi_1}, \pi_1 \pi_2) \mid f_1, f_2 \in \mathrm{Funk}(\Omega, H) \quad \pi_1, \pi_2 \in S_n \}$$

this group is called the wreath product of S_n by H [5].

As application of this paper for example we reach to the automorphism group of graph Γ_n is describe in the following figure.

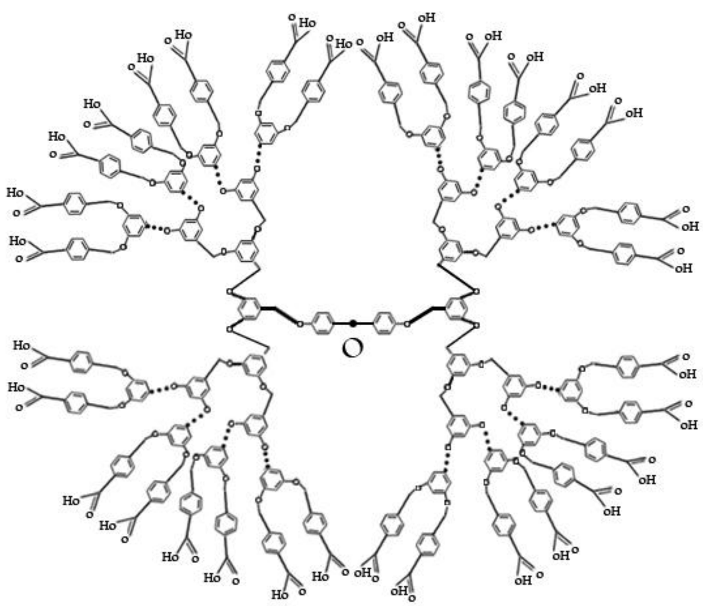


Figure1. The molecular graph of dendrimer nanostar (Γ_n)

2 MAIN RESULT AND DISSCUSSION

Definition: Let a group G acts on a set Ω and x belong to Ω then

$$G_x = \{g \in G \mid x^g = x\}$$

Lemma: Consider n ($n \geq 2$) copy of a Graph, G , and a precise vertex x in each copy. Then join them to a vertex v , and name new graph H. Then

a: $\mathrm{Aut}(H) \cong (\mathrm{Aut}(G))_x \wr S_n$

b: $|\mathrm{Aut}(H)| = |(\mathrm{Aut}(G))_x|^n . |S_n|$

Proof: Suppose Graph H is as below:

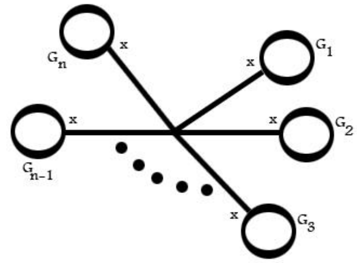


Fig 2 : The Graph (H)

Which $G_i \cong G_j$.

The group S_n acts on $\bigcup_{i=1}^{n} G_i \ \bigcup v$ with the following function :

$$\begin{cases} (G)_i{}^{\pi} = G_{(i)\pi} \\ \quad v^{\pi} = v \end{cases} \qquad \forall \quad \pi \in S_n$$

and take the comparable vertex together .

Suppose $\beta = \mathrm{Funk}(\,\Omega\ ,\ (\mathrm{Aut}(G))_x)$, where Ω={1,2,3,…,n} on $(\mathrm{Aut}(G))_x$.

$S_n|_\beta$ acts with the following function ,

$$f^{\pi}(i) = f((i)\pi) \qquad \forall\, i \in \Omega \ \ \& \ \ \pi \in S_n \ .$$

Which with this function the wreath product $\mathrm{Funk}(\Omega, (\mathrm{Aut}(G))_x) \rtimes S_n$ Can be defined as follows.

$$\overline{\beta} \quad : \{(f, 1_{S_n})\ |f \in \beta\} \qquad\qquad \overline{S_n} = \{\left(1_\beta, \sigma\right)\ |\sigma \in S_n\ \}$$

We have :

$$\overline{\beta}\,.\,\overline{S_n} \quad \cong \beta \rtimes S_n$$

So we have:

$\beta = \mathrm{Funk}(\Omega, (\mathrm{Aut}(G))_x) \rtimes S_n \ \cong \ (\left(\mathrm{Aut}(G)\right)_x \times \left(\mathrm{Aut}(G)\right)_x \times \ldots \times \ ((\mathrm{Aut}(G))_x) \rtimes \quad S_n \qquad \cong$ $(\mathrm{Aut}(G))_x \rtimes S_n$.

and

$$(Aut(G))_x \wr S_n \ \leq \ Aut(H).$$

n

for the converse of the lemma , suppose that $\varphi \in Aut(H)$. So φ has a rotation f in $\{(Aut(G_i))_x \ \ |i \in 1,2,\ldots,n\}$ and has a permutation σ which $\sigma(G_i) = G_j$ j={1,2,…,n}).

So we have,

$$\varphi = (f, 1_{S_n}).\left(1_\beta, \sigma\right) \in \overline{\beta}\,.\overline{S_n} \quad = \ (Aut(G))_x \wr S_n$$

and

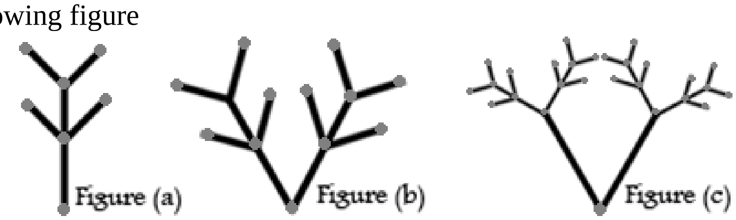
$$Aut(H) \ \leq \ (Aut(G))_x \wr S_n$$

which complete the proof of (a).

see [4] for the proof of b.

3 AUTOMORPHISM GROUP OF (Γ_n)

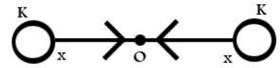
Consider the following figure

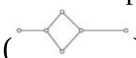
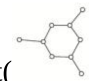
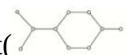


Automorphism group of the graph in Figure(a) is $z_2 \times z_2$, so by lemma automorphism group of the graph in Figure (b) is $z_4 \wr s_2$, using lemma again automorphism group of the graph of Figure(c), is $(z_4 \wr \ s_2) \ \wr s_2$. Repeating this process n times, we have the group $(z_4 \wr \ s_2) \ \wr \ s_2 \ \wr \ \ldots \wr \ \ s_2 \ \wr \ s_2 \cong Aut(H_n)$.

So the following recursive formula is generatad:

$$Aut(H_n) = Aut(H_{n-1}) \times Aut(H_{n-1}) \rtimes S_2$$

With respect to the lemma automorphism group of (

) is $(z_2 \times (Aut(K))_x) \ \wr S_2$. Now attention that The automorphism group of graph () is isomorphic with The automorphism group of graph ()with respect to symmetries and similarly Aut() ≅ Aut() and Aut() ≅ Aut() .

On the other hand the Automorphism groups of Figure 3 and Figure 4 are obviously isomorph and the automorphism group Fig 3 is isomorph with Automorphism groups of the graph (Γ_n). So that

$$Aut(\Gamma_n) \ = \ (z_4 \wr s_2) \wr s_2 \wr \ldots \wr \ \ s_2 \wr s_2.) \times z_2 \ \times z_2$$

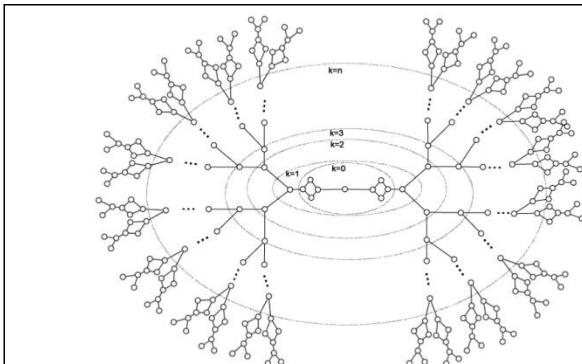
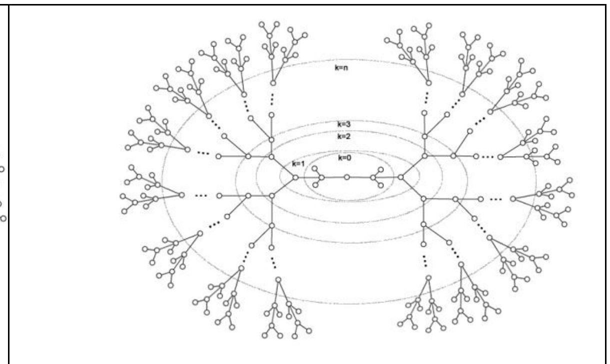
	

Figure 3. The Forth Generation Of Dendrimer Molecule (η_1)	Figure 4. The Forth Generation Of Dendrimer Molecule (η_2)

4 CONCLUSION

In this paper a general method for computing the automorphism group of a molecule is presented, which is useful for hyperbranched compounds. Our method is general and it can compute the automorphism group to other dendrimers and nanostar.

REFERENCES

1. F. Isaure, P. A. G. Cormack and D. D. Sherrington, (2006), Reactive & Functional Polymers 6665-79.
2. H. Meier and M. Lehmann, Angew. (1998), Chem.. Int. Ed. 37643-645.
3. N. C. Beck Tan, L. Balogh, S. F. Trevino, D. A. Tomalia and J. S. Lin, (1999), Polymer 402537-2545.
4. J. D. Dixon, B.M0ritmer, Book Permutation groups, Springer,44-47.
5. D. J. S. Robinson, A course in the theory of groups, Second edition. Springer- Verlag New York 1996.
6. A.R. Ashrafi and M.R. Ahmadi, (2005), Automorphism Group and Topological Indices

Of the Chemical Graph of Fullerenes, The Internet Journal of Nanotechnology,
7. M. Schönert, H.U. Besche, Th. Breuer, F. Celler, B. Eick, V. Felsch, A. Hulpke, J. Mnich, W. Nickel, G. Pfeiffer, U. Polis, H. Theißen and A. Niemeyer: GAP, Groups, Algorithms and Programming, Lehrstuhl De für Mathematik, RWTH, Aachen, 1995
8. A. R. Ashrafi: (2005),On Non-Rigid Group Theory For Some Molecules, MATCH Commun. Math. Comput. Chem., Vol. 53, (2005), 161-174.
9. A.R. Ashrafi and M. Hamadanian: "Symmetry Properties of Some Chemical Graphs", Croat. Chem. Acta, Vol. 78, pp. 159-163.

10. K. Balasubramanian: (1995), "Graph-Theoretical Perception of Molecular Symmetry", Chem. Phys. Letters, Vol. 232, pp. 415-423.
11. K. Balasubramanian: "The Symmetry Groups of Chemical Graphs", Int. J. Quant. Chem., Vol. 21, (1982), pp. 411-418.
12. M. R. Darafsheh, A. R. Ashrafi, A. Darafsheh, (2007), Non-Rigid Group Theory for 2,3-Dimethylbutane, MATCH Commun Math Comput Chem, 58(1), 47�56
13. M.R. Darafsheh, Y. Farjami, A.R. Ashrafi and M. Hamadanian, (2007), Full Non-Rigid Group of Sponge and Pina, J. Math. Chem., 41(3), 315�326
14. M.R. Darafsheh, A.R. Ashrafi and A. Darafsheh, (2006), The Full Non-Rigid Group of Hexamethylbenzene Using Wreath Product, Chem. Phys. Letters, 421.
15. M.R. Darafsheh, Y. Farjami and A.R. Ashrafi, (2005), The Non-Rigid Group of Tetraamine Platinum(II) as a Wreath Product, Bulletin of the Chemical Society of Japan, 78(6) , 996�1000.
16. M.R. Darafsheh, Y. Farjami and A.R. Ashrafi, (2005), Computing the Full Non-Rigid Group of Tetranitrocubane and Octanitrocubane Using Wreath Product, MATCH Commun. Math. Comput. Chem., 54(1), 53�74
17. M. R. Darafsheh, A. R. Ashrafi and A. Darafsheh, (2008), The Symmetry Group of Non-Rigid Tetramethylsilane, Int J Quantum Chem, 108(3), 440- 446.

Web sites:
Web-1: http://www.cjche.ca/submissioninstructions.htm, consulted 5 July 2009.
Web-2: http://www.fisher.com/instruments.htm, consulted 18 July 2009.