STUDIA UBB CHEMIA, LIX, 1, 2014 (p. 201-205)
(RECOMMENDED CITATION)

COMPUTING THE HARARY INDEX OF A CLASS OF NANOSTAR DENDRIMERS

NAHID YAVARI[a], HOSSEIN SHABANI[a,*], HAMID REZA FAZLOLLAHI[a], MIRCEA V. DIUDEA[b]

ABSTRACT. The Harary index of a molecular graph *G* is defined as the summation of the terms $1/d_G(u,v)$ where $d_G(u,v)$ is the topological distance between *u* and *v* of *G*. The aim of this paper is to compute Harary index of a class of nanostar dendrimers by using a group theoretical method.

***Keywords*:** *Graph automorphism, Harary index, dendrimer*.

INTRODUCTION

Dendrimers are hyper-branched synthetic polymers (i.e. macromolecules) with a well-defined molecular topology [1-6]. Dendrimer chemistry was first introduced in 1978 by Vogtle [1]. He synthesized the first “cascade molecule”. In 1985, Tomalia synthesized the first family of dendrimers [3]. Diudea and Katona have characterized the topology of dendrimers [7]. The topological study of these macromolecules is the aim of this article.

Let *G* be a molecular graph with the vertex set *V*(*G*) representing atoms and the edge set *E*(*G*) collecting the chemical bonds (*uv*) that join the atoms *u* and *v* in the molecular graph. The length of the shortest path between two vertices is called the topological distance and is denoted by *d*(*u*,*v*); the maximum distance between the vertex *u* and any vertex *v* in *G* is named the eccentricity of *u* and is denoted *e*(*u*).

Denote by *Aut*(*G*) the automorphism group of *G*. A topological index TI is a number that is invariant under the *Aut*(*G*). A variety of TIs have been proposed for the characterization of chemical structures and used for structure-property correlations in QSPR models [8-10].

[a] *Institute of Nanoscience and Nanotechnology, University of Kashan, Kashan 87317-51167, I.R. Iran. * Corresponding Author: shabai@grad.kashanu.ac.ir*
[b] *Faculty of Chemistry and Chemical Engineering, Babes-Bolyai University, 400028 Cluj-Napoca, Romania*

In particular, the Harary index of a graph, *H*(*G*), has been introduced in 1993, independently by Ivanciuc *et al*. [11] and by Plavšić *et al*. [12]. Even earlier, the QSAR group in Timisoara, Romania, particularly Ciubotariu [13], have used this index to express the decay of interaction between pairs of atoms in molecules as the distance between them increases. It has been named in the honor of Frank Harary, on the occasion of his 70th birthday. The Harary index is defined as follows:

$$H(G) = \sum_{u,v \in V(G)} \frac{1}{d_G(u,v)}$$

where the summation runs over all unordered pairs of vertices of the graph *G* and $d_G(u,v)$ denotes the topological distance between any two vertices *u* and *v* of *G* (i.e., the number of edges in a shortest path connecting *u* and *v*). Mathematical properties and some applications of *H,* the reader can find in refs [14-21].

In this paper, we use a group theoretical method [22-26] for computing the Harary index of the nanostar dendrimer in Figure 1.

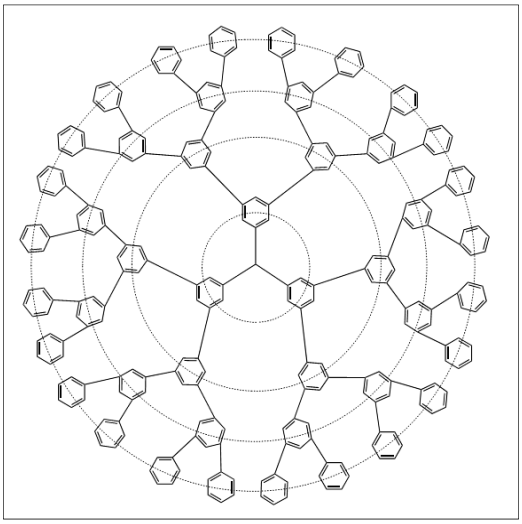

Figure 1. Molecular nanostar dendrimer *D*[4].

Throughout this paper, our notation is standard and taken mainly from the standard books of graph theory as like as [27].

MAIN RESULTS AND DISCUSSION

In this section we compute the Harary index of the dendrimer $D[n]$ (Figure 1). This dendrimer has a central vertex (denoted x_0) of degree *3* and the number of vertices and edges of $D[n]$ is equal to $|V(D[n])| = 1 + 18 \times (2^n - 1)$ and $|E(D[n])| = 21 \times (2^n - 1)$.

For a vertex v of the graph G, let $N_i(v)$ be the set of vertices at distance i (of which maximum equals $e(v)$) from v. There is a partition of the vertex set of G as $V(G) = N_0(v) \cup N_1(v) \cup \ldots \cup N_{e(v)}(v)$; it is named a *representation* of G with respect to v. Let $Rd(v) = \sum_{i=1}^{e(v)} \frac{n_i(v)}{i}$ and then rewrite the Harary index as $H(G) = \sum_{v \in V(G)} Rd(v)$.

Theorem. If the action of automorphism group of G on $V(G)$ contains the orbits $V_1, V_2, \ldots, V_k$, then $H(G) = \sum_{i=1}^{k} |V_i| Rd(v_i)$, where v_i is a vertex of the i–th orbit. In particular, if the action is transitive and v is a vertex of G then $H(G) = |V(G)| Rd(v)$.

We apply this theorem to compute the Harary index of $D[n]$. In each stage n we have 4 steps n_1 to n_4. Therefore $D[n]$ has $4n + 1$ steps and core is in step 0 ($m = 0$) of this molecule. The automorphism group of $D[n]$ is isomorphic to the wreath product $Z_2 \sim S_3$, where S_3 acts on $\Omega = \{1, 2, \ldots, 3 \times (2^n - 1)\}$. Choose the node x_0 of $D[n]$, with minimum eccentricity, as the root and suppose $x_{0,0} = x_0$. Set in the following

$$V(D[n]) = \{x_{0,0}, x_{1,1}, \ldots, x_{1,6}, \ldots, x_{3(2^n-1),1}, \ldots, x_{3(2^n-1),6}\}.$$

If automorphism group of $D[m]$ acts on $D[m]$ then the orbits are $V_0 = \{x_{0,0}\}$, $V_1 = \{x_{1,1}, x_{2,1}, x_{3,1}\}$, … , $V_{4n} = \{x_{3(2^{n-1}-1)+1,4}, \ldots, x_{3(2^n-1),4}\}$.

Let m be the number of steps in $D[n]$ and therefore $n = 4m+1$. Suppose b is the residue m module 4 and d is equal to b except $d = 4$ where $b = 0$. Denote by $\delta_{i,j}$ the Kronecker delta and define the bellow notations:

$$\Delta_d = \delta_{2,d} + \delta_{3,d}, \eta(y+t) = \frac{2^{\Delta_d}}{y+t},$$

$$\mu(x,t) = 2^{(x-1)}\left(\frac{1}{3\cdot(x-1)+t+1} + \frac{2}{3\cdot(x-1)+t+2} + \frac{2}{3\cdot(x-1)+t+3} + \frac{1}{3\cdot(x-1)+t+4}\right),$$

$$f(t,p)=\sum_{x=1}^{p}\mu(x,t)+2^{p}\sum_{y=1}^{b}\eta(y+t),$$

$$p=[\frac{k}{4}]-([\frac{m}{4}]-\delta_{4,d})-1 \text{ and } q=[\frac{m}{4}]-\delta_{4,d}.$$

Therefore for the vertex in n = 0 we have:

$$Rd(x_0)=\frac{3}{2}f(0,[\frac{k}{4}])$$

and if $n\neq 0$ then, for any vertex in row n, Rd is equals to:

$$\frac{1}{2}\sum_{m=1}^{k}3\cdot 2^{q}[2\cdot\{f(|3-d|,p)+\Delta_d f(|3-d|+2,p)+(\sum_{y=1}^{\delta_{p,-1}(k+d-2)}\frac{\eta(y)}{2^{\Delta_d}}+\delta_{2,d}(k-d))\}+$$

$$2^{\Delta_d}\{\sum_{z=1}^{q}f(d+3z-1,p+z)+2f(3q+d,[\frac{k}{4}])+\frac{1}{3q+d}+\sum_{x=1}^{q}\frac{\mu(x,d-1)}{2^{(x-1)}}+\frac{10}{3}(2^{[\frac{m}{4}]}-1)\}]$$

so, the Harary index of $D[n]$ is equal to:

$$H(D[n])=$$

$$\frac{1}{2}\{3f(0,[\frac{k}{4}])+\sum_{m=1}^{k}3\cdot 2^{q}[2\{f(|3-d|,p)+\Delta_d f(|3-d|+2,p)+(\sum_{y=1}^{\delta_{p,-1}(k+d-2)}\frac{\eta(y)}{2^{\Delta_d}}+\delta_{2,d}(k-d))\}+$$

$$2^{\Delta_d}\{\sum_{z=1}^{q}f(d+3z-1,p+z)+2f(3q+d,[\frac{k}{4}])+\frac{1}{3q+d}+\sum_{x=1}^{q}\frac{\mu(x,d-1)}{2^{(x-1)}}+\frac{10}{3}(2^{[\frac{m}{4}]}-1)\}]\}$$

In Table 1, the Harary index of $D[n]$ for some n is computed.

Table 1. Values of Harary index in dendrimers $D[n]$

n	$H(D[n])$	k	$H(D[n])$	k	$H(D[n])$	n	$H(D[n])$
1	4.5	6	163.775	11	1131.262	16	9403.148
2	19.5	7	258.443	12	1352.133	17	11508.093
3	38.9	8	291.608	13	1890.838	18	11593.067
4	56.589	9	449.681	14	3126.270	19	15747.269
5	78.168	10	788.397	15	4365.852	20	29038.085

CONCLUSIONS

The Harary index of a molecular graph G, defined as the summation of the reciprocal of topological distance between u and v of G, can be important in describing the decay of interaction between pairs of atoms in molecules as the distance between them increases. In this paper, a group theoretical method was applied to compute Harary index of a class of nanostar dendrimers.

ACKNOWLEDGEMENT

This work was partially supported by Institute of NanoSciTech of the University of Kashan.

REFERENCES

1. E. Buhleier, W. Wehner, F. Vogtle, *Synthesis*, **1978**, *2*, 155.
2. G.R. Newkombe, Z.-Q.Yao, H. Baker, V.K. Gupta, *J. Org. Chem.*,**1985**, *50*, 2003.
3. D.A. Tomalia, H. Baker, J.R. Dewald, M. Hall, G. Kallos, S. Martin, J. Roeck, J. Ryder, P.A. Smith, *Polym. J. (Tokyo),* **1985**, *17*, 117.
4. D.A. Tomalia, A.M. Naylor, W.A.I. Goddard, *Angew. Chem. Int. Ed.,* **1990**, *29*, 138.
5. C.J. Hawker, J.M.J. Frechet, *J. Am. Chem. Soc.*, **1990**, *112*, 7638.
6. E.R. Gilles, J.M.J. Frechet, *Drug Discovery Today*, **2005**, *10*, 35.
7. M.V. Diudea, G. Katona, in: G.A. Newkome, Ed., *Advan*. *Dendritic Macromol*., **1999**, *4*, 135.
8. I. Lukovits, *Int. J. Quantum.Chem.: Quantum Biology Symp*., **1992**, *19*, 217.
9. M.V. Diudea, Ed., *QSPR/QSAR Studies by Molecular Descriptors*, Nova, Huntington, N.Y., **2001**.
10. E. Estrada and E. Molina, in: M.V. Diudea*, Ed., QSPR/QSAR Studies by Molecular Descriptors,* Nova Science*,* Huntington, New York*, **2001**, 83–107.*
11. O. Ivanciuc, T.S. Balaban, and A.T. Balaban, *J. Math. Chem.,* **1993**, *12*, 309.
12. D. Plavšić, S. Nikolić, N. Trinajstić, ad Z. Mihalić, *J. Math. Chem.,* **1993**, *12*, 235.
13. D. Ciubotariu, PhD thesis, 1987, Timisoara, Romania; D. Ciubotariu, M. Medeleanu, V. Vlaia, T. Olariu, C. Ciubotariu, D. Dragos, and C. Seiman, *Molecules*, **2004**, *9*, 1053.
14. K.C. Das, B. Zhou, and N. Trinajstic, *J. Math. Chem.,* **2009**, *46*, 1369.
15. M.V. Diudea, *J. Chem. Inf. Comput. Sci*., **1997**, *37*, 292.
16. L. Feng and A. Ilic, *Appl. Math. Lett.,* **2010**, *23*, 943.
17. I. Gutman, *Indian J. Chem.,* **1997**, *36 A*, 128.
18. B. Lucić, A. Miličević, S. Nikolić, and N. Trinajstić, *Croat. Chem. Acta*, **2002**, *75*, 847.
19. K. Xu, *Discrete Appl. Math*., **2012**, *160*, 321.
20. K. Xu and K.C. Das, *Discrete Appl. Math*., **2011**, *159*, 1631.
21. B. Zhou, X. Cai, and N. Trinajstić, *J. Math. Chem*., **2008**, *44*, 611.
22. M.R. Darafsheh, *Acta. Appl. Math.,* **2010**, *110,* 1225.
23. H. Shabani, A.R. Ashrafi and M.V. Diudea, *Croat. Chem. Acta,* **2010**, *83,* 439.
24. H. Shabani, A.R. Ashrafi and I. Gutman, *Studia UBB Chemia,* **2010**, *55,* 107.
25. A.R. Ashrafi, H. Shabani, M.V. Diudea, *MATCH, Commun. Math. Comput. Chem.,* **2013**, *69,* 151.
26. A.R. Ashrafi, H. Shabani and M.V. Diudea, *Studia UBB Chemia*, **2010**, *4*, 137.
27. F. Buckley, F. Harary, *Addison-Wesley, Reading*, *MA,* **1990**.