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Kirchhoff index of the nanostar dendrimer NS[n]

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The resistance distance r(u,v) between vertices u and v of a connected (molecular) graph G is computed as the effective resistance between nodes u and v in the corresponding network constructed from G by replacing each edge of G with a unit resistor. The Kirchhoff index Kf(G) is the sum of resistance distances between all pairs of vertices. In this work, an explicit closed-form formula for Kirchhoff index of the nanostar dendrimer NS[n] is derived according to a recursive relation of resistance distances, and the Kirchhoff index of NS[n] is approximately to 7/9 of its Wiener index and 7/15 of its detour index, respectively.

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1. Introduction

A topological index is a numerical quantity derived in a unambiguous manner from the structure graph of a molecule. As a graph structural invariant, i.e., it does not depend on the labeling or the pictorial representation of a graph. Despite the considerable loss of information by compressing in a single number of a whole structure, such descriptors found broad applications in prediction of several molecular properties and biological activities. These studies called QSPR/QSAR have both diagnostic and prognostic abilities and aimed to elucidate the relation between the structure of a molecule and its properties or biological activities.

On the basis of electrical network theory, Klein and Randic [1] introduced the concept of resistance distance. Let G be a connected (molecular) graph with vertex set $V=\{v_1, v_2, ..., v_n\}$. They view G as an electrical network N by considering each edge of G as a unit resistor, then the resistance distance between vertices v_i and v_j, denoted by $r(v_i, v_j)$, is defined to be the effective resistance between nodes v_i and v_j as computed with Ohm's law in N. The Kirchhoff index [1] of G, denoted by Kf(G), is the sum of resistance distances between all pairs of vertices in G, i.e., $Kf(G)=\sum_{\{v_i,v_j\}\subseteq V} r(v_i,v_j)=\frac{1}{2}\sum_{v\in V} r(v)$, where $r(v)=\sum_{u\in V} r(v,u)$.

The Wiener index W(G) [2] is the sum of distances between pairs of vertices in G, i.e., $W(G)=\sum_{\{v_i,v_j\}\subseteq V} d(v_i,v_j)=\frac{1}{2}\sum_{v\in V} d(v)$, where $d(v_i, v_j)$ is the distance between vertices v_i and v_j and $d(v)=\sum_{u\in V} d(v,u)$. Klein and Randic [1] showed that $Kf(G)\le W(G)$ with equality if and only if G is a tree. Like Wiener index, Kirchhoff index is a structure descriptor. But it is difficult to implement some algorithms [1, 3-6] to compute resistance distance and Kirchhoff index in a graph from their computational complexity. Hence, it makes sense to find closed-from formulae for the Kirchhoff index. To this end, closed-form formulae or numerical values for Kirchhoff index have been given for some classes of graphs [7-14].

Dendrimers [15] are highly branched macromolecules. They can be precisely designed and manufactured for a wide variety of applications, such as nanotechnology, drug delivery, gene delivery, diagnostics and other fields. The first dendrimers were made by divergent synthesis approaches by Vogtle [16] in 1978. Dendrimers thereafter experienced an explosion of scientific interest because of their unique molecular architecture. The aim of this article is computing the resistance distances and Kirchhoff index of an infinite class of dendrimers. We encourage the reader to consult papers [17-26] for computing other topological indices of some dendrimers.

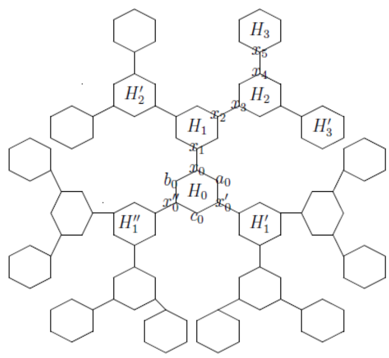

Fig. 1. The nanostar dendrimer NS[n=3].

2. Results and discussion

In this section, we will first give a recursive relation of resistance distances, and then obtain an explicit closed-form formula for Kirchhoff index of the nanostar dendrimer NS[n], depicted in Fig. 1, where n denotes the step of growth in this type of dendrimer. It is easy to see that the number of vertices and the number of edges in NS[n] are $|V| = 18\times 2^n - 12$ and $|E| = 21\times 2^n - 15$.

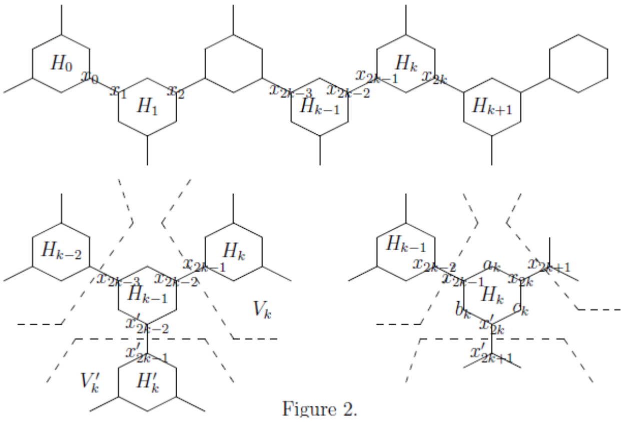

Figure 2.

Let H_0 be the central hexagon of NS[n]. H_k is a hexagon in the k-th generation, $x_{2k-2}x_{2k-1}$ is the edge connecting H_{k-1} and H_k, $V(H_k)=\{x_{2k-1}, x_{2k}, x'_{2k}, a_k, b_k, c_k\}$, $1 \le k \le n$, depicted in Figs. 2. G_k is the component containing v_{2k-1} of NS[n]-$x_{2k-2}x_{2k-1}$, $V_k=V(G_k)$ and $|V_k| = 6\times 2^{n-k+1} - 6$.

For any $x \in V$, $r(x) = \sum_{y\in V} r(x,y)$, $r(x_{2k-1}, x_{2k-2})=1$, then

$$r(x_{2k-1}) - r(x_{2k-2}) = \sum_{y\in V_k}(r(x_{2k-1},y) - r(x_{2k-2},y)) + \sum_{y\notin V_k}(r(x_{2k-1},y) - r(x_{2k-2},y))$$
$$= -|V_k| + (|V| - |V_k|) = |V| - 2|V_k|$$

i.e.,
$$r(x_{2k-1}) = r(x_{2k-2}) + |V| - 2|V_k| \tag{1}$$

In particular,

$$r(x_1) = r(x_0) + |V| - 2|V_1| = r(x_0) + 3\times 2^{n+1}.$$

$$r(x_{2k-2}) - r(x_{2k-3}) = \sum_{y\in V_k}(r(x_{2k-2},y) - r(x_{2k-3},y)) + \sum_{y\in V_k'}(r(x_{2k-2},y) - r(x_{2k-3},y))$$
$$+ \sum_{y\notin V_{k-1}}(r(x_{2k-2},y) - r(x_{2k-3},y)) + \sum_{y\in V(H_{k-1})}(r(x_{2k-2},y) - r(x_{2k-3},y))$$
$$= -\frac{4}{3}|V_k| + 0 + \frac{4}{3}(|V| - |V_{k-1}|) + 0$$
$$= \frac{4}{3}(|V| - |V_k| - |V_{k-1}|)$$

i.e.,
$$r(x_{2k-2}) = r(x_{2k-3}) - \frac{4}{3}(|V| - |V_k| - |V_{k-1}|) \tag{2}$$

From (1) and (2), we have

$$r(x_{2k-1}) = r(x_{2k-3}) + \frac{7}{3}|V| - \frac{10}{3}|V_k| - \frac{4}{3}|V_{k-1}| = r(x_{2k-3}) + 21\times 2^{n+1} - 9\times 2^{n-k+3}$$
$$= r(x_{2k-5}) + (21\times 2^{n+1} - 9\times 2^{n-k+4}) + (21\times 2^{n+1} - 9\times 2^{n-k+3}) = \cdots$$
$$= r(x_1) + 21(k-1)\times 2^{n+1} - 9\times 2^{n-k+3}(1 + 2 + 2^2 + \cdots + 2^{k-2})$$
$$= r(x_1) + (21k - 39)\times 2^{n+1} + 9\times 2^{n-k+3}$$
$$= r(x_0) + (21k - 36)\times 2^{n+1} + 9\times 2^{n-k+3}$$

i.e.,
$$r(x_{2k-1}) = r(x_0) + (21k - 36)\times 2^{n+1} + 9\times 2^{n-k+3} \tag{3}$$

and

$$r(x_{2k-2}) = r(x_{2k-1}) - |V| + 2|V_k| = r(x_0) + (21k - 45)\times 2^{n+1} + 3\times 2^{n-k+5} \tag{4}$$

$$r(a_k) - r(x_{2k-1}) = r(b_k) - r(x_{2k-1})$$
$$= \sum_{y\notin V_k}(r(a_k,y) - r(x_{2k-1},y)) + \sum_{y\in V_{k+1}}(r(a_k,y) - r(x_{2k-1},y))$$
$$+ \sum_{y\in V_{k+1}'}(r(a_k,y) - r(x_{2k-1},y)) + \sum_{y\in V(H_k)}(r(a_k,y) - r(x_{2k-1},y))$$
$$= \sum_{y\notin V_k} r(a_k, x_{2k-1}) + \sum_{y\in V_{k+1}}(r(a_k,x_{2k}) - r(x_{2k-1},x_{2k}))$$
$$+ \sum_{y\in V_{k+1}'}(r(a_k,x_{2k}') - r(x_{2k-1},x_{2k}')) + 0$$
$$= \frac{5}{6}(|V| - |V_k|) - \frac{1}{2}|V_{k+1}| + \frac{1}{6}|V_{k+1}'| = \frac{5}{6}(|V| - |V_k|) - \frac{1}{3}|V_{k+1}|$$

i.e.,
$$r(a_k) = r(b_k) = r(x_{2k-1}) + \frac{5}{6}(|V| - |V_k|) - \frac{1}{3}|V_{k+1}|.$$

And by (3),

$$r(a_k) = r(b_k) = r(x_0) + (42k - 57)\times 2^n + 15\times 2^{n-k+2} - 3 \tag{5}$$

Similarly,

$$r(c_k) - r(x_{2k-1})$$
$$= \sum_{y\notin V_k}(r(c_k,y) - r(x_{2k-1},y)) + \sum_{y\in V_{k+1}}(r(c_k,y) - r(x_{2k-1},y))$$
$$+ \sum_{y\in V_{k+1}'}(r(c_k,y) - r(x_{2k-1},y)) + \sum_{y\in V(H_k)}(r(c_k,y) - r(x_{2k-1},y))$$
$$= \sum_{y\notin V_k} r(c_k, x_{2k-1}) + \sum_{y\in V_{k+1}}(r(c_k,x_{2k}) - r(x_{2k-1},x_{2k}))$$
$$+ \sum_{y\in V_{k+1}'}(r(c_k,x_{2k}') - r(x_{2k-1},x_{2k}')) + 0$$
$$= \frac{3}{2}(|V| - |V_k|) - \frac{1}{2}|V_{k+1}| - \frac{1}{2}|V_{k+1}'| = \frac{3}{2}(|V| - |V_k|) - |V_{k+1}|$$

i.e.,
$$r(c_k) = r(x_{2k-1}) + \frac{3}{2}(|V| - |V_k|) - |V_{k+1}|.$$

And by (3),

$$r(c_k) = r(x_0) + (42k - 45)\times 2^n + 3\times 2^{n-k+4} - 3 \tag{6}$$

From (3)-(6), we have

$$r(H_k) = \sum_{y\in V(H_k)} r(y) = r(x_{2k-1}) + r(x_{2k}) + r(x_{2k}') + r(a_k) + r(b_k) + r(c_k)$$
$$= [r(x_0) + (21k - 36)\times 2^{n+1} + 9\times 2^{n-k+3}] + 2[r(x_0) + (21k - 24)\times 2^{n+1} + 3\times 2^{n-k+4}]$$
$$+ 2[r(x_0) + (42k - 57)\times 2^n + 15\times 2^{n-k+2} - 3] + [r(x_0) + (42k - 45)\times 2^n + 3\times 2^{n-k+4} - 3]$$
$$= 6r(x_0) + (252k - 327)\times 2^n + 21\times 2^{n-k+4} - 9$$

Now, we compute $r(x_0)$.

$$r(x_0, x_{2k-1}) = r(x_0, x_1) + r(x_1, x_2) + r(x_2, x_3) + r(x_3, x_4) + \cdots + r(x_{2k-2}, x_{2k-1})$$
$$= 1 + \frac{4}{3} + 1 + \frac{4}{3} + \cdots + 1 = \frac{7}{3}k - \frac{4}{3}$$

$$r(x_0,b_k)=r(x_{0,}a_k)=r(x_{0,}x_{2k-1})+r(x_{2k-1,}a_k)=\frac{7}{3}k-\frac{4}{3}+\frac{5}{6}=\frac{7}{3}k-\frac{1}{2}$$

$$r(x_0,x_{2k}^{'})=r(x_{0,}x_{2k})=r(x_{0,}x_{2k-1})+r(x_{2k-1,}x_{2k})=\frac{7}{3}k-\frac{4}{3}+\frac{4}{3}=\frac{7}{3}k$$

$$r(x_0,c_k)=r(x_{0,}x_{2k-1})+r(x_{2k-1,}c_k)=\frac{7}{3}k-\frac{4}{3}+\frac{3}{2}=\frac{7}{3}k+\frac{1}{6}$$

So, $r(x_0,H_k)=\sum_{y\in H_k}r(x_0,y)=14k-\frac{13}{6}$,

and $\sum_{y\in V_1}r(x_0,y)=\sum_{k=1}^{n}2^{k-1}r(x_0,H_k)=\sum_{k=1}^{n}(14k-\frac{13}{6})2^{k-1}$

By the symmetry of NS[n], we have

$$\sum_{y\in V_1^{'}}r(x_0^{'},y)=\sum_{y\in V_1^{''}}r(x_0^{''},y)=\sum_{y\in V_1}r(x_0,y)=\sum_{k=1}^{n}(14k-\frac{13}{6})2^{k-1}$$

And,

$$\begin{aligned}r(x_0)&=\sum_{y\in V_1}r(x_0,y)+\sum_{y\in V_1^{'}}(r(x_0^{'},y)+r(x_0,x_0^{'}))++\sum_{y\in V_1^{''}}(r(x_0^{''},y)+r(x_0,x_0^{''}))+\sum_{y\in V(H_0)}r(x_0,y)\\&=3\sum_{y\in V_1}r(x_0,y)+r(x_0,x_0^{'})|V_1^{'}|+r(x_0,x_0^{''})|V_1^{''}|+\sum_{y\in V(H_0)}r(x_0,y)\\&=3\sum_{k=1}^{n}(14k-\frac{13}{6})\times 2^{k-1}+2\times\frac{4}{3}\times 6(2^n-1)+\frac{35}{6}\\&=\frac{1}{6}(63n\times 2^{n+2}-195\times 2^n+230)\end{aligned}$$

$$\begin{aligned}Kf(NS[n])&=\frac{1}{2}[r(H_0)+\sum_{k=1}^{n}(3\times 2^{k-1}\times r(H_k))]\\&=\frac{1}{2}[6r(x_0)+9(2^n-1)+\sum_{k=1}^{n}(3\times 2^{k-1}(6r(x_0)+(252k-327)\times 2^n+21\times 2^{n-k+4}-9))]\\&=\frac{1}{2}[6(3\times 2^n-2)r(x_0)+9(2+191\times 2^n-193\times 4^n+28n\times 2^{n+1}+84n\times 4^n)]\\&=\frac{1}{2}[(3\times 2^n-2)(63n\times 2^{n+2}-195\times 2^n+230)+9(2+191\times 2^n-193\times 4^n+28n\times 2^{n+1}+84n\times 4^n)]\\&=189n\times 4^{n+1}-1161\times 4^n+2799\times 2^{n-1}-221\end{aligned}$$

Theorem. The Kirchhoff index of NS[n] is

$$Kf(NS[n])=189n\times 4^{n+1}-1161\times 4^n+2799\times 2^{n-1}-221.$$

In [21], Karbasioun, Ashrafi and Diudea gave the Wiener index and detour index of NS[n]:

$$W(NS[n])=486(2n-3)\times 2^{2n}+1755\times 2^n-270,$$
$$dd(NS[n])=2619\times 2^n+(1620n-2214)\times 2^{2n}-342.$$

It can obtained that the Kirchhoff index of NS[n] is approximately to 7/9 of its Wiener index and 7/15 of its detour index:

$$\lim_{n\to\infty}\frac{Kf(NS[n])}{W(NS[n])}=\frac{7}{9},\qquad \lim_{n\to\infty}\frac{Kf(NS[n])}{dd(NS[n])}=\frac{7}{15}$$

and the convergence rate is fast.

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References

[1] D. J. Klein, M. Randic, J. Math. Chem. **12,** 81 (1993).
[2] H. J. Wiener, J. Amer. Chem. Soc. **69,** 17 (1947).
[3] D. J. Klein, H. Y. Zhu, J. Math. Chem. **23,** 179 (1998).
[4] D. Babic, D. J. Klein, I. Lukovits, S. Nikolic, N. Trinajstic, Int. J. Quantum Chem. **90,** 166 (2002).
[5] R. B. Bapat, I. Gutman, W. J. Xiao, Z. Naturforsch **58a,** 494 (2003).
[6] D. J. Klein, Croat. Chem. Acta **75,** 633 (2002).
[7] J. L. Palacios, Int. J. Quantum Chem. **81,** 135 (2001).
[8] W. Zhang, H. Deng, MATCH Commun. Math. Comput. Chem. **61,** 683 (2009).
[9] Q. Guo, H. Deng, MATCH Commun. Math. Comput. Chem. **61,** 713 (2009).
[10] H. Deng, MATCH Commun. Math. Comput. Chem. **63,** 171 (2010).
[11] H. Zhang, Y. Yang, Int. J. Quantum Chem. **107,** 330 (2007).
[12] Y. J. Yang, X. Y. Jiang, MATCH Commun. Math Comput. Chem. **60,** 107 (2008).
[13] H. Zhang, X. Jiang, Y. Yang, MATCH Commun. Math. Comput. Chem. **61,** 697 (2009).
[14] Y. Yang, H. Zhang, Int.J. Quantum Chem. **108,** 503 (2008).
[15] M. V. Diudea, G. Katona, Advan. Dendritic Macromol. **4**, 135 (1999).
[16] E. Buhleier, W. Wehner, F. Vogtle, Synthesis **2**, 155 (1978).
[17] S. Alikhani, M. A. Iranmanesh, J. Comput. Theor. Nanosci. **7**, 2314 (2010).
[18] M. H. Khalifeh, M. R. Darafsheh, H. Jolany, J. Comput. Theor. Nanosci. **8**, 220 (2011).
[19] M. B. Ahmadi, M. Seif, Digest Journal of Nanomaterials and Biostructures **5**, 335 (2010).
[20] H. Wang, H. Hua, Digest Journal of Nanomaterials and Biostructures **5**, 497 (2010).
[21] A. Karbasioun, A. R. Ashrafi, M. V. Diudea, MATCH Commun. Math. Comput. Chem. **63,** 239 (2010).
[22] A. Karbasioun, Ali Reza Ashrafi, Journal of Chemistry and Chemical Engineering **28,** 49 (2009).
[23] A. R. Ashrafi, K. Amini, Optoelectron. Adv. Mater.-Rapid Commun. **4**(6), 877 (2010).
[24] A. R. Ashrafi, M. Saheli, Optoelectron. Adv. Mater. –Rapid Commun. **4**(6), 898 (2010).
[25] A. R. Ashrafi, A. Seyed Mirzaei, G. H. Fath-Tabar, Optoelectron. Adv. Mater. - Rapid Commun. **4**(12), 2194 (2010).
[26] G. H. Fath-Tabar, A. R. Ashrafi, Optoelectron. Adv. Mater. –Rapid Commun. **5**(1), 96 (2011).

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