Atom-Bond Connectivity and Geometric Arithmetic Indices of Dendrimer Nanostars

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Abstract

Let *G* be a molecular graph. The atom-bond connectivity (*ABC*) and geometric-arithmetic (*GA*) indices of *G* are defined as $ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$ and $GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$, where d_u (or d_v) denoted the degree of the vertex *u* (or *v*), respectively. A dendrimer is a hyperbranched molecule built up from branched units called monomers. In this paper, the *ABC* and *GA* indices for two families of dendrimer nanostars are presented.

Keywords: *Atom-bond connectivity, Geometric-arithmetic, Dendrimer, Graph*

1 Introduction and Preliminaries

A simple graph *G* = (*V*,*E*) is a finite nonempty set *V*(*G*) of objects called vertices together with a (possibly empty) set *E*(*G*) of unordered pairs of distinct vertices of *G* called edges. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds.

A graphical invariant is a number related to a graph which is structural invariant, that is to say it is fixed under graph automorphisms. In chemistry and for chemical graphs, these invariant numbers are known as the topological indices. There are many publications on the topological indices. One of the most important topological indices is the Randic index [15]. But a great variety of physico-chemical properties rest on factors rather than branching. In order to take this into consideration, Estrada et al. proposed a new index, know as the atom-bond connectivity (*ABC*) index[9] of graph *G*, which is abbreviated as *ABC*(*G*). The *ABC*(*G*) is defined as $\sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$, where d_u (or d_v) the degree the vertex *u* (or *v*).

The *ABC* index keeps the spirit of Randic index, and it provides a good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes [9,10]. The properties of *ABC* index for trees have been studied in [12,17]. More mathematical properties for the *ABC* index may be found in some papers [4,5,6,7,11].

Vukicevic and Furtula [16] proposed a topological index named the geometric-arithmetic (*GA*) index. The *GA* index is defined as defined as $\sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$, where d_u (or d_v) the degree of the vertex *u* (or *v*). For comprehensive survey of this index, the reader is refered to [8] and references therein.

Dendrimers are hyper-branched macromolecules, with a rigorously tailored architecture. They can be synthesized, in a controlled manner, either by a divergent or a convergent procedure. Dendrimers have gained a wide range of applications in supra-molecular chemistry, particularly in host guest reactions and self-assembly processes. Their applications in chemistry, biology and nano-science are unlimited. Recently, the topological indices of some dendrimer nanostars have been investigated in [1,2,3,13,14].

In this paper, we continue to investigate the *ABC* and *GA* indices of two families of dendrimer nanostars. As by-product, four formulas are obtained for computing the *ABC* and *GA* indices of these families of dendrimers.

2 Main Results

We first give some examples of the *ABC* and *GA* indices for some simple graphs. Let P_n, C_n, K_n, O_n and S_n be the path, cycle, complete, empty and star graphs with *n* vertices.

Example 2.1 For $n \geq 3$

1. $ABC(P_n) = \frac{\sqrt{2}}{2}(n-1)$.
2. $ABC(C_n) = \frac{\sqrt{2}}{2}n$.
3. $ABC(K_n) = \frac{\sqrt{2}}{2}n\sqrt{n-2}$.

Example 2.2

1. For every $n \geq 1, GA(O_n) = 0$.
2. For every $n \geq 1, GA(K_n) = \binom{n}{2}$.
3. For every $n \geq 1, GA(S_n) = \frac{2(n-1)^{3/2}}{n}$.

Now we consider the molecular graph $G(n) = D_1[n]$, where *n* is the steps of growth in this kind of dendrimer of generation 1-3. Figure 1 shows first kind of dendrimer of generation 1-3 with 4 growth stages, $D_1[4]$ Note that $D_1[n]$ can be divided to 2^n hexagonal in each step (stage). Define d_{ij} to be the number of edges connecting a vertex of degree *i* with a vertex of degree *j*. Let denote a vertex of degree *i* with *i*-vertex, and an edge connecting a *j*-vertex with a *k*-vertex by (*j*,*k*)-edge. By simple calculation, we have $|V(D_1[n])| = 2^{n+4} - 9$ and $|E(D_1[n])| = 18 \times 2^n - 11$([1]).

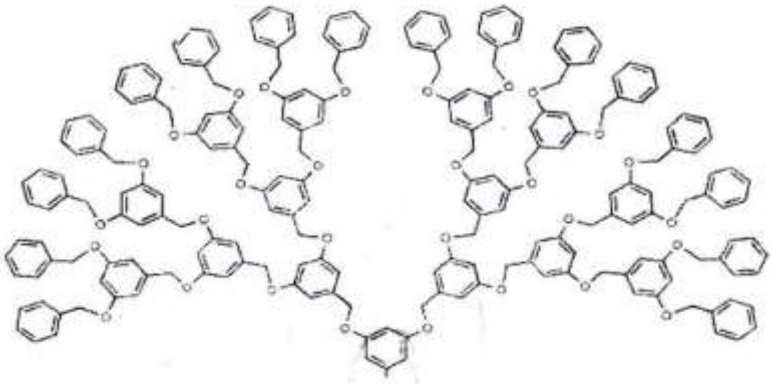

Figure 1: The first kind of dendrimer of generation 1-3 with 4 growth stages, $D_1[4]$

Theorem 2.1 Let $n \in N$. Then, the atom bond connectivity (*ABC*) of the graph $D_1[n]$] is given as
$ABC(D_1[n]) = (\frac{1}{\sqrt{3}} + 9 \times 2^n - 6)\sqrt{2}$

Proof. For the graph $D_1[n]$ which contributes (1,3), (2,2) and (2,3)-edges, the formula of *ABC* index can be deduced to

$$ABC(D_1[n]) = \frac{\sqrt{2}}{\sqrt{3}} d_{13} + \frac{\sqrt{2}}{2} d_{22} + \frac{\sqrt{2}}{2} d_{23}$$

There is only one (1,3)-edge in the kernel of $D_1[n]$ ($n = 0$) (see Figure 2), so d_{13} =1for all steps of growth. By induction argument, we obtain $d_{22} = 2^{n+2} + 2(2^n - 1) = 6 \times 2^n - 2$. Note that d_{23} =$|E(D_1[n])|$-(d_{13} +d_{22}) and $|E(D_1[n])| = 18 \times 2^n - 11$. So, we have d_{23}= $12 \times 2^n - 10$. Table 1 shows the values of d_{ij} where (*i,j*)= (1,3), (2,2),(2,3) and *n* = 1,2,3,4.

Hence,

$$ABC(D_1[n]) = \frac{\sqrt{2}}{\sqrt{3}}(1) + \frac{\sqrt{2}}{2}(6 \times 2^n - 2) + \frac{\sqrt{2}}{2}(12 \times 2^n - 10) = (\frac{1}{\sqrt{3}} + 9 \times 2^n - 6)\sqrt{2}$$

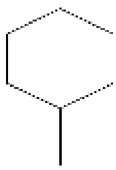

Figure 2: The kernel of $D_1[n]$

Table 1: The values of d_{ij} in $D_1[n]$ where (*i,j*)= (1,3), (2,2),(2,3)

Stages / d_{ij}	1	2	3	4
d_{13}	1	1	1	1
d_{22}	10	22	46	94
d_{23}	14	38	86	182

Now the proof is complete. □

Theorem 2.2 Let $n \in N$. Then, the geometric-arithmetic (*GA*) of the graph $D_1[n]$ is given as
$GA(D_1[n]) = \left(\frac{24}{5}\sqrt{6} + 6\right)2^n + \frac{\sqrt{3}}{2} - 4\sqrt{6} - 2.$

Proof. For the graph $D_1[n]$ which contributes (1,3), (2,2) and (2,3)-edges, the formula of *GA* index can be deduced to

$$GA(D_1[n]) = \frac{\sqrt{3}}{2} d_{13} + d_{22} + \frac{2}{5} d_{23}.$$

By Theorem 2.1, we know that d_{13} =1, d_{22} = $6 \times 2^n - 2$ and d_{23}= $12 \times 2^n - 10$.

Hence, we have

$$GA(D_1[n]) = \frac{\sqrt{3}}{2}(1) + (6 \times 2^n - 2) + \frac{2}{5}\sqrt{6}(12 \times 2^n - 10)$$
$$= \left(\frac{24}{5}\sqrt{6} + 6\right)2^n + \frac{\sqrt{3}}{2} - 4\sqrt{6} - 2$$

This completes the proof. □

Now we consider another molecular graph *G*(*n*) = *D*3[*n*], where *n* is the steps of growth in this kind of dendrimer of generation 1-3. Figure 3 shows the first kind of dendrimer of generation 1-3 with 3 growth stages, $D_3[3]$.

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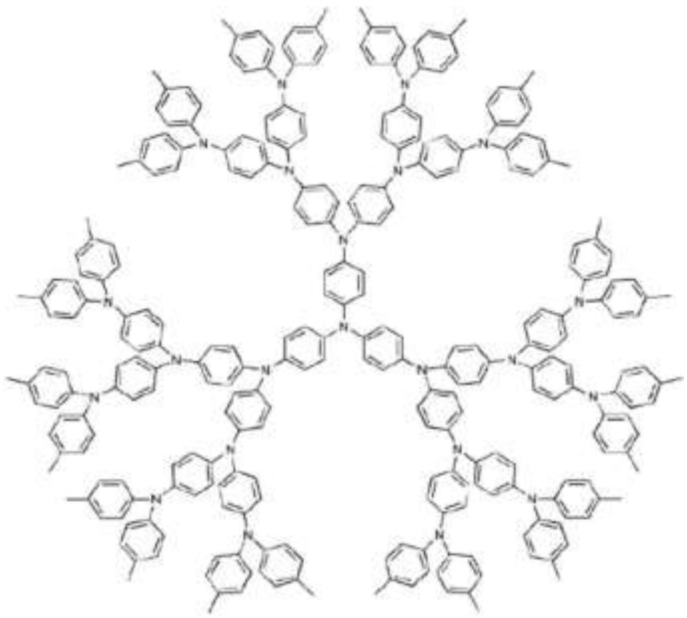

Figure 3: The first kind of dendrimer of generation 1-3 with 3 growth stages, D_3[3]

Theorem 2.3 Let $n \in N$. Then, the atom bond connectivity (*ABC*) of the graph D_3[3] is given as
$ABC(D_3[n]) = \left(18\sqrt{2} + \sqrt{6} + 6\right)2^n - 9\sqrt{2} - 4$

Proof. For the graph $D_3[n]$ which contributes (1,3), (2,2), (2,3) and (3,3)-edges, the formula of *ABC* index can be deduced to

$ABC(D_3[n]) = \frac{\sqrt{6}}{3}d_{13} + \frac{\sqrt{2}}{2}d_{22} + \frac{\sqrt{2}}{2}d_{23} + \frac{2}{3}d_{33}$

By induction argument, we can show that d_{13} =3×2^n, d_{22} = $12 \times 2^n - 6$, d_{23}= $24\times 2^n - 12$ and d_{33} = $9 \times 2^n - 6$. Table 2 shows the values of d_{ij} where (*i,j*)= (1,3), (2,2),(2,3),(3,3) and n = 1,2,3 therefore,

$ABC(D_3[n]) = \frac{\sqrt{6}}{3}(3 \times 2^n) + \frac{\sqrt{2}}{2}(12 \times 2^n - 6) + \frac{\sqrt{2}}{2}(24 \times 2^n - 12) + \frac{2}{3}(9 \times 2^n - 6)$
= $\left(18\sqrt{2} + \sqrt{6} + 6\right)2^n - 9\sqrt{2} - 4$

Table 2: The values of d_{ij} in $D_3[n]$ where (*i,j*)= (1,3), (2,2), (2,3) and (3,3).

d_{ij} \ Stage	1	2	3
d_{13}	6	12	24
d_{22}	18	42	90
d_{23}	36	84	180
d_{33}	12	30	66

This completes the proof. □

Theorem 2.4 Let $n \in N$. Then, the geometric-arithmetic (*GA*) of the graph $D_3[n]$ is given as
$GA(D_3[n]) = \left(21 + \frac{3}{2}\sqrt{3} + \frac{48}{5}\sqrt{6}\right)2^n - 12 - \frac{24}{5}\sqrt{6}.$

Proof. For the graph $D_3[n]$ which contributes (1,3), (2,2), (2,3) and (3,3)-edges, the formula of *GA* index can be deduced to

$GA(D_3[n]) = \frac{\sqrt{3}}{2}d_{13} + d_{22} + \frac{2}{5}d_{23} + d_{33}.$

By Theorem 2.3, we know that d_{13} = 3×2^n, d_{22} = $12\times 2^n - 6$, d_{23}= $24 \times 2^n - 12$ and d_{33} = $9 \times 2^n - 6$. Hence, we have

$GA(D_3[n]) = \frac{\sqrt{3}}{2}(3 \times 2^n) + (12 \times 2^n - 6) + \frac{2}{5}\sqrt{6}(24 \times 2^n - 12) + (9 \times 2^n - 6)$
= $\left(21 + \frac{3}{2}\sqrt{3} + \frac{48}{5}\sqrt{6}\right)2^n - 12 - \frac{24}{5}\sqrt{6}.$

This completes the proof. □

Remarks

This paper deals with the computation of the atom bond connectivity (*ABC*) and geometric arithmetic (*GA*) indices for some nanostar dendrimers. The problem on *ABC* and *GA* indices of nanostructures and general graphs is remains open for further investigation.

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مؤشرات اتصال الذرة–الآصرة والحسابية الهندسية للدندرايمر النانوية

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الملخص

ليكن G بيان جزيئي. تعرف مؤشرات اتصال الذرة–الاصرة (ABC) والحسابية الهندسية (AG) كالتالي: $ABC(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}$ و $GA(G)=\sum_{uv\in E(G)}\frac{2\sqrt{d_ud_v}}{d_u+d_v}$.
حيث ان d_u و d_v هي درجات الرؤوس u و v على التوالي. الدندرايمر هو تشعب جزيء متراكم من وحدات متفرعة تسمى مونومرات. في هذه البحث اوجدنا مؤشرات ABC و AG لعائلتين من الدندرايمرات النانوية.