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Research Article

Computing Different Versions of Atom-bond Connectivity Index of Dendrimers

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Abstract. Atom-bond connectivity index has a prominent place among the topological indices because it is excellently correlated with the thermodynamic properties of alkanes, especially with their heats of formation. In this paper, we compute closed formulae of different versions of ABC index of two classes of perylenediimide-cored dendrimers.

Keywords. Atom-bond connectivity index; Perylenediimide-cored dendrimers; Molecular graph

MSC. 68Qxx

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1. Introduction

A dendrimer consists of an initiative core, interior layer (which is composed of repeating units that are attached to the initiative core) and the exterior layer which is attached to the outermost interior generations. Dendrimers have very well-defined nanostructures and high-level control over its size, branching density and surface functionality. Due to small size, easy uptake by cells (through endocytosis) and other unique properties, dendrimers can be conjugated to various chemical species, such as detection agents, targeting components, imaging agents, pharmaceutical, biomolecules, affinity ligands, radio ligands and for various bioanalytical applications [14]. Dendrimers are currently attracting the interest of a great number of scientists because of their unusual chemical and physical properties and the wide range of potential application in different fields such as biology, medicine, physics, chemistry and engineering [17].

Topological indices are numerical invariants which are associated with molecular graph structure that correlate various physical properties, chemical reactivity or biological activity with the chemical structure. Top(G) denotes a topological index of a graph G and if H is another graph such that $G \cong H$ then Top(G) = Top(H). In different fields such as chemistry, biochemistry and nanotechnology,different topological indices are found to be useful in isomer discrimination, structure-property relationship and structure-activity relationship. Various topological indices have been defined so for. Throughout this paper, G will be a molecular graph with vertex set $V(G)$ and edge set $E(G)$. Vertices of G correspond to atoms and edges correspond to chemical bonds between atoms.Two vertices u and v of G are adjacent if they are end vertices of an edge and we write $e = vu$ or $e = uv$.For a vertex u the set of neighbor vertices is denoted by N_u and is defined as $N_u = \{v \in V(G) : uv \in E(G)\}$. The degree of a vertex $u \in V(G)$ is denoted by d_u and is defined as the number of vertices incident to u. Let S_u denotes the sum of the degrees of all neighbors of vertex u, that is, $S_u = \sum_{v \in N_u} d_v$. The line graph $L(G)$ of a graph G has the vertex set $V(L(G)) = E(G)$, where the two vertices of $L(G)$ are adjacent if and only if the corresponding edges of G are adjacent.

The atom-bond connectivity index (henceforth, ABC index) comes from the Randić connectivity index which was introduced by Milan Randić [16] in 1975. Randić connectivity index reflects the molecular branching. However, many physico-chemical properties are dependent on other factors rather than branching. In order to take this into account, Estrada et al. [5] defined ABC index. In 2008, Estrada [6] gave the justification theory of this index. After this, the interest in the study of ABC index has grown rapidly. This index reflects important structural properties of graphs in general. The ABC index has attracted significant attention from researchers in the last two decay and the chemical and mathematical properties of ABC index were extensively studied [2, 4, 8, 9].

The ABC index of a molecular graph G is defined as:

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}. \tag{1.1}$$

The fourth member of the class of ABC index was introduced by Ghorbani and Hosseinzadeh [11] in 2010 and defined as:

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}. \tag{1.2}$$

The edge version of ABC index was introduced by Farahani [7] in 2013 and defined as:

$$ABC_e(G) = \sum_{uv \in E(L(G))} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}. \tag{1.3}$$

For more details on ABC index, the reader is referred to [3, 10, 12].

The water-soluble PDI-cored dendrimers have a prominent place among the other dendrimers due to their wide range of potential application in different fields. The water-soluble PDI-cored dendrimers have many advantages include excellent photo stability, high quantum yield, low cytotoxicity, versatile surface modification and strong red fluorescence. These dendrimers have broad biological applications including gene delivery, fluorescence live-cell imaging and fluorescent labelling [15]. Husin et al. [13] calculated the ABC index of some nanostar dendrimers. Bokhary and his co-authors [1] have discussed this index for certain classes of dendrimers. In this paper, we compute different versions of ABC index of two classes of PDI-cored dendrimers.

2. Different Versions of *ABC* Index of Dendrimers

Let $D_1(n)$ be the molecular graph of first type of PDI-cored dendrimer, where n represents the generation stage of $D_1(n)$. The $D_1(n)$ with $n = 0$ and $n = 1$ are shown in Figure 1. $D_1(n)$ and $n = 3$ are shown in Figure 2. The order of $D_1(0)$ is 30 and size is 36. The order of $D_1(0)$ for $n \geq 1$ is given by $|V(D_1(n))| = 20(2^n + 1)$.

The size of $D_1(n)$ for $n \geq 1$ is given by $|E(D_1(n))| = 2(5 \times 2^{n+1} + 13)$.

In this section, we compute closed formulae of ABC and $ABCD_4$ indices of dendrimers.

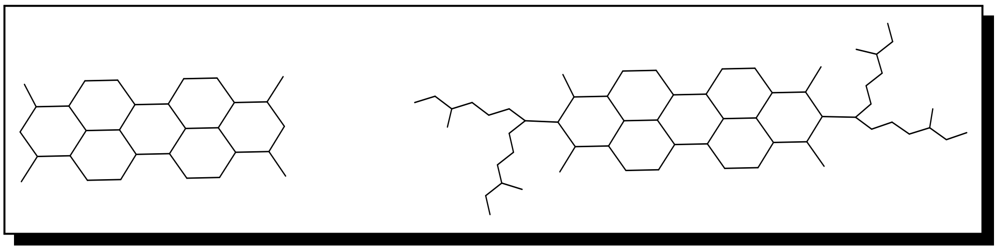

Figure 1. From left to right: $D_1(n)$ with $n = 0$ and $n = 1$, respectively

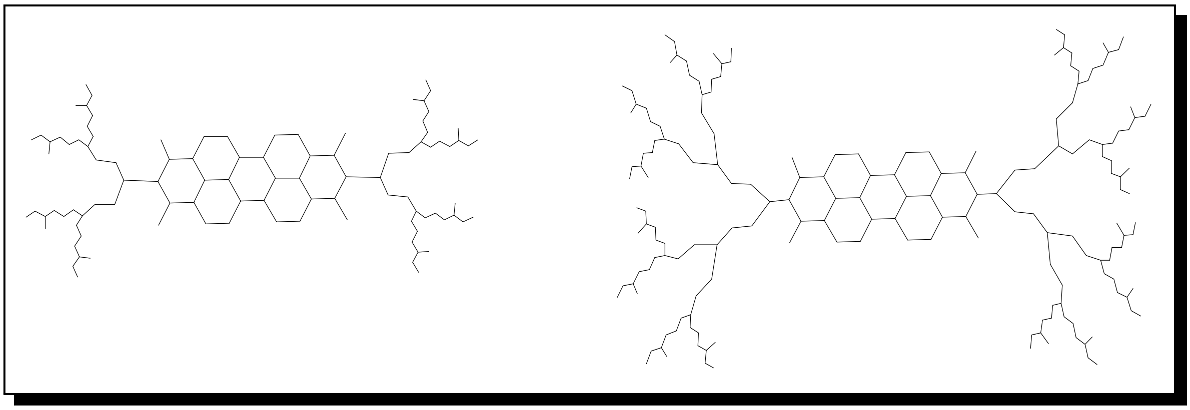

Figure 2. From left to right: $D_1(n)$ with $n = 2$ and $n = 3$, respectively

Table 1. Edge partition of graph $D_1(n)$ based on degree of end vertices of each edge

(d_u, d_v), $uv \in E(D_1(n))$	Number of edges for $n = 0$	Number of edges for $n \geq 1$
$(1,2)$	0	2^{n+1}
$(1,3)$	4	$2^{n+1} + 4$
$(2,2)$	4	$3 \times 2^{n+1}$
$(2,3)$	8	$5 \times 2^{n+1}$
$(3,3)$	20	22

Theorem 2.1. *For the graph $D_1(n)$, the ABC index is given by*

$$ABC(D_1(n)) = \begin{cases} \dfrac{12\sqrt{\frac{2}{3}}+36\sqrt{\frac{1}{2}}+40}{3}, & n=0; \\ \dfrac{12\times 2^{n+\frac{1}{2}}+60\times 2^{n-\frac{3}{2}}+4\sqrt{6}(2^{n-1}+1)+44}{3}, & n\geq 1. \end{cases}$$

Proof. There are two cases to discuss while proving this result. Firstly, we prove this result for $n=0$. The edge partition based on the degree of end vertices of each edge of the graph $D_1(n)$ is given in Table 1. By using the values of Table 1 for $n=0$ in (1.1), we get

$$ABC(D_1(0)) = (0)\sqrt{\frac{1+2-2}{1\times 2}}+(4)\sqrt{\frac{1+3-2}{1\times 3}}+(4)\sqrt{\frac{2+2-2}{2\times 2}}+(8)\sqrt{\frac{2+3-2}{2\times 3}} +(20)\sqrt{\frac{3+3-2}{3\times 3}}.$$

After some simplifications, we have

$$ABC(D_1(0)) = \frac{12\sqrt{\frac{2}{3}}+36\sqrt{\frac{1}{2}}+40}{3}.$$

Now, we prove this result for $n\geq 1$. By using the values of Table 1 for $n\geq 1$ in (1.1), we obtain

$$ABC(D_1(n)) = 2^{n+1}\sqrt{\frac{1+2-2}{1\times 2}}+(2^{n+1}+4)\sqrt{\frac{1+3-2}{1\times 3}}+(3\times 2^{n+1})\sqrt{\frac{2+2-2}{2\times 2}} +(5\times 2^{n+1})\sqrt{\frac{2+3-2}{2\times 3}}+22\sqrt{\frac{3+3-2}{3\times 3}}.$$

After some simplifications, we have

$$ABC(D_1(0)) = \frac{12\times 2^{n+\frac{1}{2}}+60\times 2^{n-\frac{3}{2}}+4\sqrt{6}(2^{n-1}+1)+44}{3}.$$ □

In $D_1(0)$, there are total 30 vertices on the degree based sum of neighbor vertices, among which 4 vertices are of degree 3, 8 vertices are of degree 5, 4 vertices are of degree 7, 8 vertices are of degree 8 and 6 vertices are of degree 9. In $D_1(n)$, for $n\geq 1$, there are total $20(2^n+1)$ vertices on the degree based sum of neighbor vertices, among which 2^{n+1} vertices are of degree 2, $4(2^{n-1}+1)$ vertices are of degree 3, 2^{n+2} vertices are of degree 4, $5\times 2^{n-1}$ vertices are of degree 5, $4(2^{n-1}-1)$ vertices are of degree 6, 6 vertices are of degree 7, 8 vertices are of degree 8 and 9 vertices are of degree 9. There are eight types of edges on degree based sum of neighbor vertices of each edge in $D_1(0)$ and there are thirteen types of edges on degree based sum of neighbor vertices of each edge in $D_1(n)$ for $n\geq 1$. We will use these partitions of edges to calculate ABC_4 index. Table 2 gives such types of edges of $D_1(n)$. Now by the help of Table 2, we compute the ABC_4 index in the following theorem.

Theorem 2.2. *For the graph $D_1(n)$, the ABC_4 index is given by*

$$ABC_4(D_1(n))\begin{cases}\sqrt{\frac{26}{7}+\frac{8}{9}+\frac{\sqrt{14}\times 105+\sqrt{42}\times 160}{420}+\frac{\sqrt{110}\times 168+\sqrt{30}\times 280+\sqrt{2}\times 1232}{420}}, & n=0;\\ \frac{2^n(5\sqrt{10}+10\sqrt{2}+5\sqrt{7}+8\sqrt{10}+15\sqrt{3})}{5\sqrt{5}}+\frac{207\sqrt{5}+96\sqrt{15}+16\sqrt{70}+120\sqrt{21}}{18\sqrt{70}}+\frac{72\sqrt{35}+36\sqrt{65}+72\sqrt{77}}{18\sqrt{70}}, & n\ge 1.\end{cases}$$

Table 2. Edge partition of graph $D_n(n)$ based on degree sum of neighbor vertices of end vertices of each edge

(s_u,s_v), $uv\in E(D_1(n))$	Number of edges for $n\ge 1$	Number of edges for $n=0$	(s_u,s_v)	Number of edges for $n\ge 1$	Number of edges for $n=0$
$(2,4)$	2^{n+1}	0	$(5,8)$	8	8
$(3,5)$	2^{n+1}	0	$(7,8)$	4	4
$(3,7)$	4	4	$(7,9)$	6	4
$(4,5)$	$3\times 2^{n+1}$	0	$(8,8)$	2	2
$(5,5)$	2^{n+2}	4	$(8,9)$	8	8
$(5,6)$	$3(2^{n+1}-4)$	0	$(9,9)$	2	2
$(5,7)$	4	0			

Proof. We find the edge partition of the graph $D_1(n)$ based on degree sum of vertices lying at unit distance from end vertices of each edge in Table 2. Firstly, we prove this result for $n=0$. By using the values of Table 2 for $n=0$ in (1.2), we get

$$ABC_4(D_1(0))=(4)\sqrt{\frac{3+7-2}{3\times 7}}+(4)\sqrt{\frac{5+5-2}{5\times 5}}+(8)\sqrt{\frac{5+8-2}{5\times 8}}+(4)\sqrt{\frac{7+8-2}{7\times 8}}+(4)\sqrt{\frac{9+7-2}{9\times 7}}+(2)\sqrt{\frac{8+8-2}{8\times 8}}+(8)\sqrt{\frac{9+8-2}{9\times 8}}+(2)\sqrt{\frac{9+9-2}{9\times 9}}.$$

After some simplifications, we have

$$ABC_4(D_1(0))=\sqrt{\frac{26}{7}+\frac{8}{9}+\frac{\sqrt{14}\times 105+\sqrt{42}\times 160+\sqrt{110}\times 168+\sqrt{30}\times 280+\sqrt{2}\times 1232}{420}}.$$

Now, we prove this result for $n\ge 1$. By using the values of Table 2 for $n\ge 1$ in (1.2), we obtain

$$ABC_4(D_1(n))=2^{n+1}\sqrt{\frac{2+4-2}{2\times 4}}+2^{n+1}\sqrt{\frac{3+5-2}{3\times 5}}+4\sqrt{\frac{3+7-2}{3\times 7}}+(3\times 2^{n+1})\sqrt{\frac{4+5-2}{4\times 5}}+2^{n+2}\sqrt{\frac{5+5-2}{5\times 5}}+3(2^{n+1}-4)\sqrt{\frac{5+6-2}{5\times 6}}+4\sqrt{\frac{5+7-2}{5\times 7}}+8\sqrt{\frac{5+8-2}{5\times 8}}$$

$$+4\sqrt{\frac{7+8-2}{7\times8}}+6\sqrt{\frac{7+9-2}{7\times9}}+8\sqrt{\frac{8+9-2}{8\times9}}+2\sqrt{\frac{8+9-2}{8\times9}}+2\sqrt{\frac{9+9-2}{9\times9}}.$$

After some simplifications, we have

$$\begin{aligned}ABC_4(D_1(n)) &= \frac{2^n(5\sqrt{10}+10\sqrt{2}+15\sqrt{7}+8\sqrt{10}+15\sqrt{3})-30\sqrt{3}}{5\sqrt{5}}\\ &\quad+\frac{207\sqrt{5}+96\sqrt{15}+16\sqrt{70}+120\sqrt{21}+72\sqrt{35}+36\sqrt{65}+72\sqrt{77}}{18\sqrt{70}}.\end{aligned}$$ □

Let $D_2(n)$ be the molecular graph of second type of PDI-cored dendrimer, where n represents the generation stage of $D_2(n)$. The $D_2(n)$ with $n=0$ is shown in Figure 3. $D_2(n)$ with $n=1$ and $n=2$ are shown in Figure 4. The order of $D_2(0)$ is 94 and size is 106. The order of $D_2(n)$ for $n \geq 1$ is given by $|V(D_2(n))| = 2(68\times 2^n - 21)$.

The size of $D_2(n)$ for $n \geq 1$ is given by $|E(D_2(n))| = 136\times 2^n - 30$.

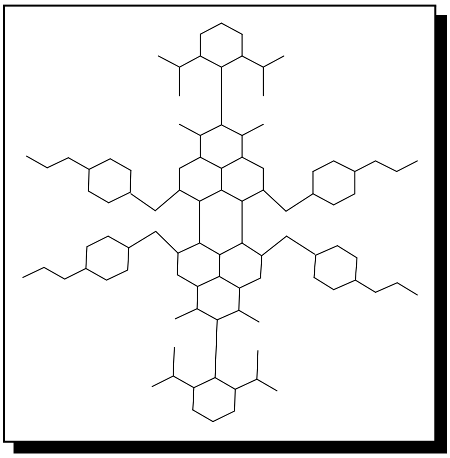

Figure 3. $D_2(n)$ with $n=0$

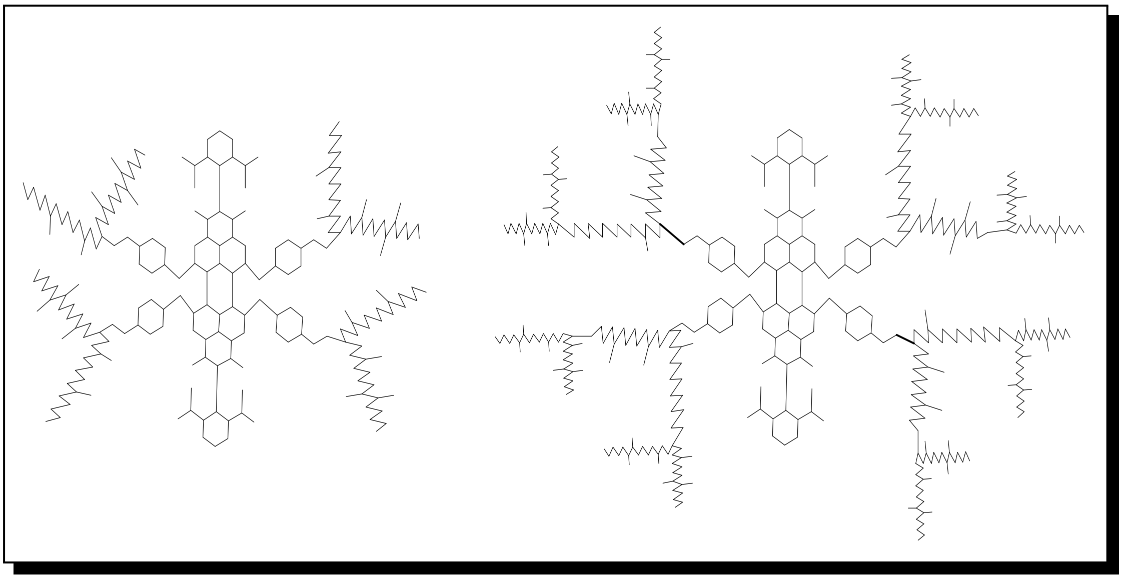

Figure 4. From left to right: $D_2(n)$ with $n=1$ and $n=2$, respectively

Table 3. Edge partition of graph $D_2(n)$ based on degree of end vertices of each edge

(d_u, d_v), $uv \in E(D_2(n))$	Number of edges for $n = 0$	Number of edges for $n \geq 1$
(1,2)	0	2^{n+2}
(1,3)	12	$24 \times 2^n - 12$
(2,2)	16	$8(7 \times 2^n - 5)$
(2,3)	44	$4(11 \times 2^n - 1)$
(3,3)	34	$8 \times 2^n + 26$

Theorem 2.3. *For the graph $D_2(n)$ the ABC index is given by*

$$ABC(D_2(n)) = \begin{cases} \dfrac{36\sqrt{\frac{2}{3}} + 180\sqrt{\frac{1}{2}} + 68}{3}, & n = 0; \\ \dfrac{4\left(2^n + 78\sqrt{\frac{1}{2}} - 33\sqrt{\frac{1}{2}} + 2^n \times 4 + 2^n \times 18\sqrt{\frac{2}{3}} + 13 - 9\sqrt{\frac{2}{3}}\right)}{3}, & n \geq 1. \end{cases}$$

Proof. There are two cases to discuss while proving this result. Firstly, we prove this result for $n = 0$. The edge partition based on the degree of end vertices of each edge of the graph $D_2(n)$ is given in Table 3. By using the values of Table 3 for $n = 0$ in (1.1), we get

$$ABC(D_2(0)) = (12)\sqrt{\frac{1+3-2}{1\times 3}} + (16)\sqrt{\frac{2+2-2}{2\times 2}} + (44)\sqrt{\frac{2+3-2}{2\times 3}} + (34)\sqrt{\frac{3+3-2}{3\times 3}}.$$

After some simplifications, we have

$$ABC(D_2(0)) = \frac{36\sqrt{\frac{2}{3}} + 180\sqrt{\frac{1}{2}} + 68}{3}.$$

Now, we prove this result for $n \geq 1$. By using the values of Table 3 for $n \geq 1$ in (1.1), we obtain

$$\begin{aligned} ABC(D_2(n)) = 2^{n+2}\sqrt{\frac{1+2-2}{1\times 2}} + (24\times 2^n - 12)\sqrt{\frac{1+3-2}{1\times 3}} + (8(7\times 2^n - 5))\sqrt{\frac{2+2-2}{2\times 2}} \\ + (4(11\times 2^n - 1))\sqrt{\frac{2+3-2}{2\times 3}} + (8\times 2^n + 26)\sqrt{\frac{3+3-2}{3\times 3}}. \end{aligned}$$

After some simplifications, we have

$$ABC(D_2(n)) = \frac{4\left(2^n \times 78\sqrt{\frac{1}{2}} - 33\sqrt{\frac{1}{2}} + 2^n \times 4 + 2^n \times 18\sqrt{\frac{2}{3}} + 13 - 9\sqrt{\frac{2}{3}}\right)}{3}.$$

In $D_2(0)$ there are total 94 vertices on the degree based sum of neighbor vertices, among which 12 vertices are of degree 3, 2 vertices are of degree 4, 32 vertices are of degree 5, 20 vertices are of degree 6, 8 vertices are of degree 7, 12 vertices are of degree 9 and 8 vertices are of degree 8. In $D_2(n)$, for $n \geq 1$, there are total $136 \times 2^n - 42$ vertices on the degree based sum of neighbor vertices, among which 2^{n+2} vertices are of degree 2, $4(14 \times 2^{n-1} - 3)$ vertices are of degree 3, $32 \times 2^n - 30$ vertices are of degree 4, $4(13 \times 2^n - 6)$ vertices are of degree 5, $20 \times 2^n - 4$ vertices are of degree 6, 8 vertices are of degree 7, 8 vertices are of degree 8, 12 vertices are of degree 9.

There are thirteen types of edges on degree based sum of neighbor vertices of each edge in $D_2(0)$ and seventeen types of edges on degree based sum of neighbor vertices of each edge in $D_2(n)$ for $n \geq 1$. We will use these partitions of edges to calculate ABC_4 index. Table 4 gives such types of edges of $D_2(n)$. Now by the help of this Table, we compute the ABC_4 index in the following theorem.

Table 4. Edge partition of graph $D_2(n)$ based on degree sum of neighbor vertices of end vertices of each edge

(s_u, s_v), $uv \in E(D_2(n))$	Number of edges for $n \geq 1$	Number of edges for $n = 0$	(s_u, s_v)	Number of edges for $n \geq 1$	Number of edges for $n = 0$
$(2,3)$	2^{n+2}	0	$(5,8)$	8	8
$(3,4)$	2^{n+2}	0	$(3,7)$	4	4
$(3,5)$	2^{n+3}	8	$(6,7)$	8	8
$(3,6)$	$16(2^n - 1)$	0	$(6,8)$	4	4
$(6,6)$	$4(2^{n+1} - 1)$	4	$(7,8)$	4	4
$(4,4)$	$16(2^n - 1)$	0	$(7,9)$	8	8
$(4,5)$	$28(2^n - 1)$	4	$(8,9)$	8	8
$(5,5)$	$12(2^{n+1} - 1)$	12	$(9,9)$	10	10
$(5,6)$	$8(7 \times 2^{n-1} - 1)$	24			

Theorem 2.4. *For the graph $D_2(n)$ the ABC_4 index is given by*

$$ABC_4(D_2(n)) = \begin{cases} \sqrt{\frac{26}{7}} + 8\sqrt{\frac{11}{42}} + 8\sqrt{\frac{2}{5}} + 24\sqrt{\frac{3}{10}} \\ \quad + \frac{2(21\sqrt{35} + 20\sqrt{42} + 21\sqrt{110} + 252\sqrt{2})}{105} \\ \quad + \frac{58 + 24\sqrt{2} + 6\sqrt{10} + 6\sqrt{30}}{9}, & n = 0; \\ \frac{2^{n+1} \times 3\left(2\sqrt{\frac{3}{2}} + \sqrt{5} + 4\sqrt{\frac{6}{5}}\right) + (2^n - 1)(8\sqrt{42} + 36\sqrt{2})}{3\sqrt{3}} \\ \quad + \frac{120\sqrt{\frac{3}{2}}(2^{n-1} \times 7 - 1) + 210\sqrt{7}(2^n - 1)}{15\sqrt{5}} \\ \quad + \frac{(2^{n+1} - 1)(72\sqrt{10} + 50\sqrt{2})}{15\sqrt{5}} + \frac{24\sqrt{\frac{165}{2}} + 24\sqrt{30} + 30\sqrt{42}}{9\sqrt{35}} \\ \quad + \frac{58\sqrt{35} + 24\sqrt{70} + 9\sqrt{130} + 18\sqrt{154}}{9\sqrt{35}}, & n \geq 1. \end{cases}$$

Proof. There are two cases to discuss while proving this result. Firstly, we prove this result for $n = 0$. The edge partition based on the degree of end vertices of each edge of the graph $D_2(n)$ is given in Table 4. By using the values of Table 4 for $n = 0$ in (1.2), we get

$$
\begin{aligned}
ABC_4(D_2(0)) &= (8)\sqrt{\frac{3+5-2}{3\times 5}} + (4)\sqrt{\frac{4+5-2}{4\times 5}} + (24)\sqrt{\frac{5+6-2}{5\times 6}} + (12)\sqrt{\frac{5+5-2}{5\times 5}} \\
&\quad + (4)\sqrt{\frac{3+7-2}{3\times 7}} + (8)\sqrt{\frac{5+8-2}{5\times 8}} + (4)\sqrt{\frac{6+6-2}{6\times 6}} + (8)\sqrt{\frac{6+7-2}{6\times 7}} \\
&\quad + (4)\sqrt{\frac{6+8-2}{6\times 8}} + (4)\sqrt{\frac{7+8-2}{7\times 8}} + (8)\sqrt{\frac{7+9-2}{7\times 9}} + (8)\sqrt{\frac{8+9-2}{8\times 9}} \\
&\quad + (10)\sqrt{\frac{9+9-2}{9\times 9}}.
\end{aligned}
$$

After some simplifications, we have

$$
\begin{aligned}
ABC_4(D_2(n)) &= \sqrt{\frac{26}{7}} + 8\sqrt{\frac{11}{42}} + 8\sqrt{\frac{2}{5}} + 24\sqrt{\frac{3}{10}} + \frac{2(21\sqrt{35} + 20\sqrt{42} + 21\sqrt{110} + 252\sqrt{2})}{105} \\
&\quad + \frac{58 + 24\sqrt{2} + 6\sqrt{10} + 6\sqrt{30}}{9}.
\end{aligned}
$$

We find the edge partition of the graph $D_2(n)$ based on degree sum of vertices lying at unit distance from end vertices of each edge in Table 4. Now, we prove this result for $n \geq 1$. By using the values of Table 4 for $n \geq 1$ in (1.2), we obtain

$$
\begin{aligned}
ABC_4(D_2(n)) &= 2^{n+2}\sqrt{\frac{2+3-2}{2\times 3}} + 2^{n+2}\sqrt{\frac{3+4-2}{3\times 4}} + 2^{n+3}\sqrt{\frac{3+5-2}{3\times 5}} + 16(2^n - 1)\sqrt{\frac{3+6-2}{3\times 6}} \\
&\quad + 16(2^n - 1)\sqrt{\frac{4+4-2}{4\times 4}} + 28(2^n - 1)\sqrt{\frac{4+5-2}{4\times 5}} \quad + 12(2^{n+1} - 1)\sqrt{\frac{5+5-2}{5\times 5}} \\
&\quad + 8(7\times 2^{n-1} - 1)\sqrt{\frac{5+6-2}{5\times 6}} + 4\sqrt{\frac{3+7-2}{3\times 7}} + 8\sqrt{\frac{5+8-2}{5\times 8}} + 4(2^{n+1} - 1)\sqrt{\frac{6+6-2}{6\times 6}} \\
&\quad + 8\sqrt{\frac{6+7-2}{6\times 7}} + 4\sqrt{\frac{6+8-2}{6\times 8}} + 4\sqrt{\frac{7+8-2}{7\times 8}} + 8\sqrt{\frac{7+9-2}{7\times 9}} + 8\sqrt{\frac{8+9-2}{7\times 9}} \\
&\quad + 10\sqrt{\frac{9+9-2}{9\times 9}}.
\end{aligned}
$$

After some calculations, we get

$$
\begin{aligned}
ABC_4(D_2(n)) &= \frac{2^{n+2}\times 3\sqrt{\frac{3}{2}} + 2^{n+1}\times 3\sqrt{5} + 2^{n+3}\times 3\sqrt{\frac{6}{3}} + 8\sqrt{42}(2^n - 1) + 36\sqrt{2}(2^n - 1)}{3\sqrt{3}} \\
&\quad + \frac{120\sqrt{\frac{3}{2}}(2^{n-1}\times 7 - 1) + 72\sqrt{10}(2^{n-1} - 1) + 50\sqrt{2}(2^{n+1} - 1) + 210\sqrt{7}(2^n - 1)}{15\sqrt{5}} \\
&\quad + \frac{24\sqrt{\frac{165}{2}}24\sqrt{30} + 30\sqrt{42} + 58\sqrt{35} + 24\sqrt{70} + 9\sqrt{130} + 18\sqrt{154}}{9\sqrt{35}}. \qquad \square
\end{aligned}
$$

3. The Edge Version of *ABC* Index of Dendrimers

Let $L(D_1(n))$ be the line graph of molecular graph $D_1(n)$. The line graphs of $D_1(n)$ with $n = 1$ and $n = 2$, respectively are shown in Figure 5. The order and the size of $L(D_1(n))$ is given by

$$|V(L(D_1(n)))| = 2(5\times 2^{n+1}+13), \qquad |E(L(D_1(n)))| = 48(2^{n-1}+1).$$

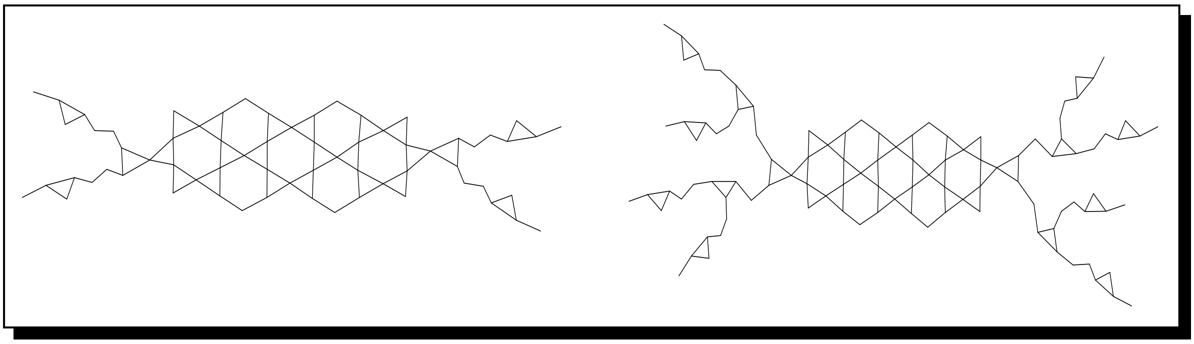

Figure 5. From left to right: the line graph of $D_1(n)$ with $n = 1$ and $n = 2$, respectively

Table 5. Edge partition of the line graph of $D_1(n)$ based on degree of end vertices of each edge

(d_u, d_v), $uv \in E(D_1(n))$	Number of edges
$(1,3)$	2^{n+1}
$(2,2)$	2^{n+1}
$(2,3)$	$3\times 2^{n+2}$
$(2,4)$	8
$(3,3)$	$2^{n+3}-10$
$(3,4)$	20
$(4,4)$	30

Theorem 3.1. *For the graph $D_1(n)$, the edge version of ABC index is given by*

$$ABC_e(D_1(n)) = \frac{2^{n+1}(21\sqrt{3}+6+8\sqrt{6})+24\sqrt{3}+30\sqrt{10}+135-20\sqrt{6}}{3\sqrt{6}}.$$

Proof. The edge partition of the line graph of $D_1(n)$ based on degree of end vertices of each edge is given in Table 5. By using Table 5 and (1.3), we have

$$\begin{aligned} ABC_e(D_1(n)) &= 2^{n+1}\sqrt{\frac{1+3-2}{1\times 3}}+2^{n+1}\sqrt{\frac{2+2-2}{2\times 2}}+(3\times 2^{n+2})\sqrt{\frac{2+3-2}{2\times 3}} \\ &\quad +8\sqrt{\frac{2+4-2}{2\times 4}}+(2^{n+3}-10)\sqrt{\frac{3+3-2}{3\times 3}}+20\sqrt{\frac{3+4-2}{3\times 4}}+30\sqrt{\frac{4+4-2}{4\times 4}}. \end{aligned}$$

After some simplifications, we get

$$ABC_e(D_1(n)) = \frac{2^{n+1}(21\sqrt{3}+6+8\sqrt{6})+24\sqrt{3}+30\sqrt{10}+135-20\sqrt{6}}{3\sqrt{6}}. \qquad \square$$

Let $L(D_2(n))$ be the line graph of molecular graph $D_2(n)$. The line graphs of $D_2(n)$ with $n = 1$ and $n = 2$, respectively are shown in Figure 6. The order and the size of $L(D_2(n))$ is given by

$$|V(L(D_2(n)))| = 136 \times 2^n - 30, \quad |E(L(D_2(n)))| = 164 \times 2^n - 6.$$

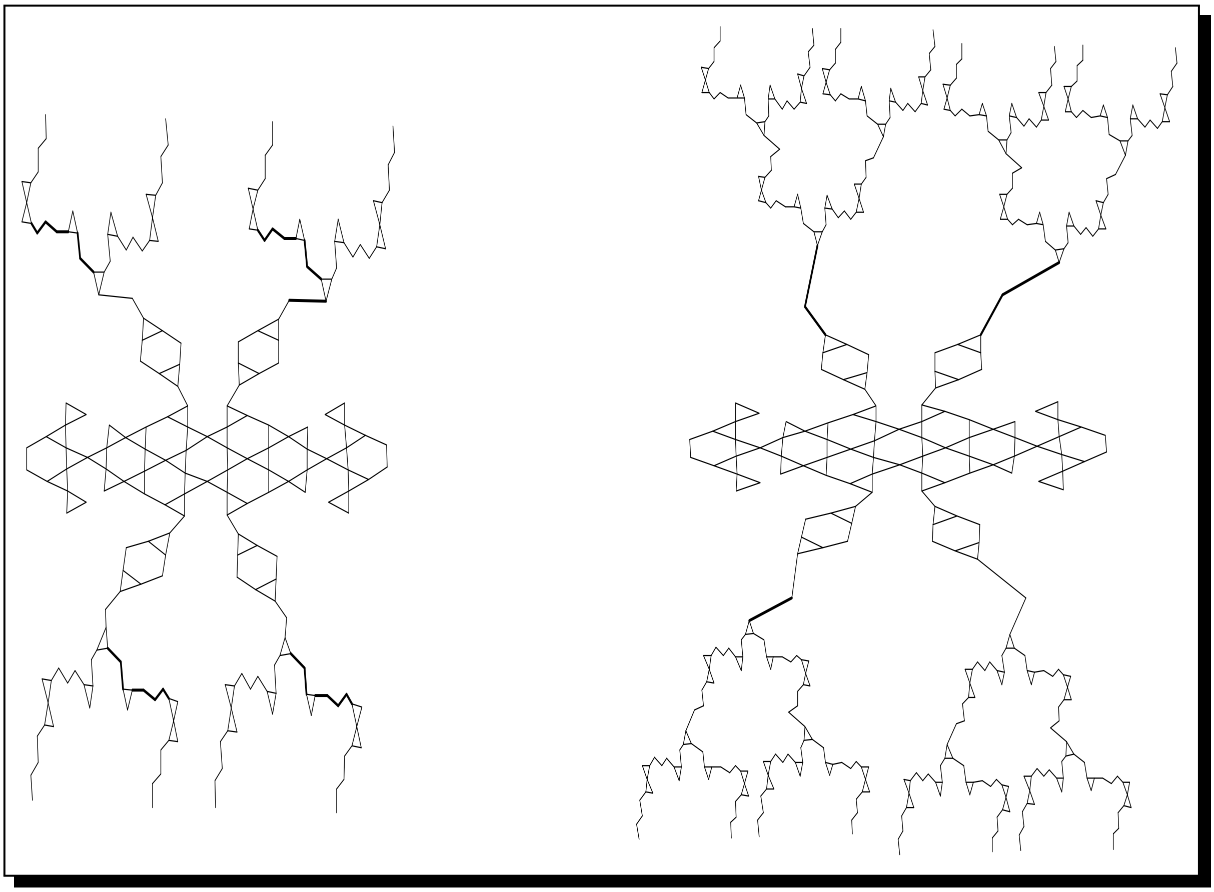

Figure 6. From left to right: the line graph of $D_2(n)$ with $n = 1$ and $n = 2$, respectively

Table 6. Edge partition of the line graph of $D_2(n)$ based on degree of end vertices of each edge

(d_u, d_v), $uv \in E(D_2(n))$	Number of edges
$(2,2)$	$9 \times 2^{n+2} - 26$
$(2,3)$	$4(19 \times 2^n - 13)$
$(2,4)$	2^{n+4}
$(3,3)$	$4(5 \times 2^n + 4)$
$(3,4)$	$2^{n+4} + 8$
$(4,4)$	48

Theorem 3.2. *For the graph $D_2(n)$, the edge version of ABC index is given by*

$$ABC_e(D_2(n)) = \frac{2^{n+4}\sqrt{\frac{3}{2}} + 4\sqrt{5}(2^{n+1}+1) + 36\sqrt{2}}{\sqrt{3}} + \frac{2^n \times 336\sqrt{\frac{1}{2}} - 234\sqrt{\frac{1}{2}} + 2^n \times 40 + 32}{3}.$$

Proof. The edge partition of the line graph of $D_2(n)$ based on degree of end vertices of each edge is given in Table 6. By using Table 6 and (1.3), we have

$$ABC_e(D_2(n)) = (9\times 2^{n+2}-26)\sqrt{\frac{2+2-2}{2\times 2}} + 4(19\times 2^n-13)\sqrt{\frac{2+3-2}{2\times 3}} + 2^{n+2}\sqrt{\frac{2+4-2}{2\times 4}}$$
$$+4(5\times 2^n+4)\sqrt{\frac{3+4-2}{4\times 4}} + (2^{n+4}+8)\sqrt{\frac{3+4-2}{3\times 4}} + 48\sqrt{\frac{4+4-2}{4\times 4}}.$$

After some simplifications, we obtain

$$ABC_e(D_2(n)) = \frac{2^{n+4}\sqrt{\frac{3}{2}}+4\sqrt{5}(2^{n+1}+1)+36\sqrt{2}}{\sqrt{3}} + \frac{2^n\times 336\sqrt{\frac{1}{2}}-234\sqrt{\frac{1}{2}}+2^n\times 40+32}{3}. \qquad \square$$

4. Conclusion

We considered two classes of PDI-cored dendrimers and studied certain versions of ABC index for their molecular graphs. It will be interesting to compute polynomials and their related indices of $D_1(n)$ and $D_2(n)$ shown in Figures 1, 2, 3, and 4.

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Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

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