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Connectivity indices of some famous dendrimers

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ABSTRACT

In the present paper,formulas for calculating topological indices (2-order connectivity index and 2-order sum-connectivity index) in three classes of dendrimers are derived.

Keywords: Vertex-degree, 2-order connectivity index, 2-order sum-connectivity index, Dendrimer

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INTRODUCTION

Dendrimer chemistry was first discovered by Fritz Vögtle and coworkers [1] in1978.Dendrimers are highly branched and reactive three-dimensional macromolecules, with successive layers or generations of branch units surrounding a central core. They are being investigated for possible uses in biology, nanotechnology, gene therapy, drug delivery, photonics, and other fields [2-6]. Chemical graph theory is an important tool for studying molecular structures. In theoretical chemistry,molecular descriptors,especially topological indices are used for modelling information of molecules, including physical,pharmacological and biological of chemical compounds. The topological study of dendrimers and nanostructures is the subject of some recent papers [7-13].

The rest of the paper organized as follows. In the second part of this work, we give the necessary definitions while the third section gives the main results; namely we determine 2-order connectivity index and 2-order sum-connectivity index for three infinite classes of dendrimers. Conclusions and references will close this article.

DEFINITIONS

Now, we gathered some notations as well as preliminary notions which will be needed for the rest of the paper.Molecules and molecular compounds are often modeled by molecular graphs. A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Let $G(V,E)$ be a connected graph, with the vertex set $V(G)$ and edge set $E(G)$.The degree (= number of first neighbors) of a vertex $u \in V(G)$ is denoted byd_u.A topological index of G is a real number related to G and it is invariant under all graph isomorphism. In chemistry, graph invariants areknown as topological indices.

In 1975, Randić first addressed the problem of relating the physical properties of alkanes to the degree of branching across an isomeric series [14]. The degree of branching of a molecule was quantified using a branching index which subsequently became known as first-order molecular connectivity indexχ. In 1986, Kier and Hall extended this to higher orders and introduced modificationsto account for heteroatoms [15].

Let$G$be a simple connected graph of order$n$. For an integer $m \geq 1$, the m-order connectivity index of an organic molecule whose molecule graph G is defined as:

$$^m\chi(G) = \sum_{i_1 \dots i_{m+1}} \frac{1}{\sqrt{d_{i_1} \dots d_{i_{m+1}}}},$$

Where $i_1 \dots i_{m+1}$(for simplicity) runs over all paths of length m in $G$and d_i denote the degree of vertex u_i. In 2009, Zhou and Trinajstić [16] proposed another connectivity index, named the sum-connectivity index. It has been found that the sum-connectivity index correlates well with π-electronic energy of benzenoid hydrocarbons, and it is frequently applied in quantitative structure property and structure-activity studies. The m-order sum-connectivity index of G is defined as:

$$^{m}X(G) = \sum_{i_1 \cdots i_{m+1}} \frac{1}{\sqrt{d_{i_1} + \cdots + d_{i_{m+1}}}}.$$

2-order connectivity index is defined as follows:

$$^{2}\chi(G) = \sum_{i_1 i_2 i_3} \frac{1}{\sqrt{d_{i_1} d_{i_2} d_{i_3}}}.$$

2-order sum-connectivity index is defined as follows:

$$^{2}X(G) = \sum_{i_1 i_2 i_3} \frac{1}{\sqrt{d_{i_1} + d_{i_2} + d_{i_3}}}.$$

We encourage the reader to consult papers [17-20]for further study on this topic. Here, our notation is standard and mainly taken from standard books of chemical graph theory such as, e.g., [21-22].

RESULTS AND DISCUSSION

In this section, we discuss two topological descriptors, namely 2-order connectivity and 2-order sum-connectivity indicesfor three classes of dendrimers. For a review, historical details and further bibliography see refs. [23-24].

Results for first type of dendrimer

Consider the molecular graph of light-harvesting dendrimer$D_1[n]$ depicted in Figure 1. Here n is the step of growth in the type of dendrimer. The vertex and edge cardinalities are $|V(D_1[n])| = 39 \times 2^{n+1} + 15$ and $|E(D_1[n])| = 23 \times 2^{n+2} + 18$ respectively.

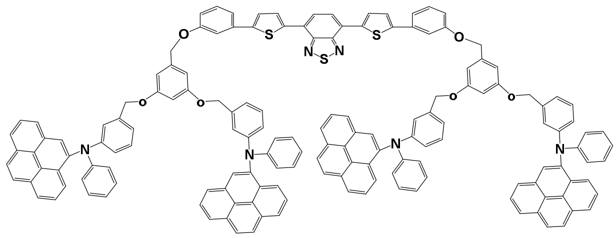

Figure 1:Light-harvesting dendrimer$D_1[n]$ for $n = 1$

Theorem 1. The 2-order connectivity index of $D_1[n]$ is calculated as:

$$^{2}\chi(D_1[n]) = 2^n\left(\frac{28\sqrt{2}}{3} + \frac{115\sqrt{3}}{9}\right) + \frac{15\sqrt{2}}{4} + \frac{7\sqrt{3}}{9}.$$

Proof. Let we define d_{ijk} as a number of 2-edges paths with 3 vertices of degree i, $j$and k, respectively. It is obvious,d_{ijk}= d_{kji}. First, we define d_{222} to be the number of edges connecting the three vertices of degree 2, 2 and 2 (The red path), $d_{223}$to be the number of edges connecting the three vertices of degree 2, 2 and 3 (The blue path),$d_{232}$to be the number of edges connecting the three vertices of degree 2, 3 and 2 (The orange path), d_{323} to be the number of edges connecting three vertices of degree 3, 2 and 3 (The green path),d_{233} to be the number of edges connecting three vertices of degree 2, 3 and 3 (The yellow path),$d_{333}$to be the number of edges connecting the three vertices of degree 3 (The pink path).

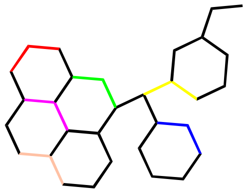

Figure 2: Examples of 2-edges pathsof a particular of $D_1[n]$

Table 1: Categorization all 2-edges paths on based their first and end point and the number of these path

2-edges paths	$D_1[1]$	$D_1[2]$	$D_1[3]$	...	$D_1[n]$
$(2,2,2)$	27	51	99	...	$3\times 2^{n+2}+3$
$(2,2,3)$	64	120	232	...	$7\times 2^{n+2}+8$
$(2,3,2)$	62	130	266	...	$17\times 2^{n+1}-6$
$(3,2,3)$	18	38	78	...	$5\times 2^{n+1}-2$
$(2,3,3)$	76	132	244	...	$7\times 2^{n+2}+20$
$(3,3,3)$	48	92	180	...	$11\times 2^{n+1}+4$

To prove the theorem, we apply induction on n. Table 1 shows the data for the above discussed edge partition of $D_1[n]$. Now we apply the formula of $^2\chi$index to compute this index for$D_1[n]$.Since

$$^2\chi(D_1[n]) = \sum_{i_1 i_2 i_3} \frac{1}{\sqrt{d_{i_1} d_{i_2} d_{i_3}}},$$

then

$$^2\chi(D_1[n]) = \frac{3\times 2^{n+2}+3}{\sqrt{2\times 2\times 2}} + \frac{7\times 2^{n+2}+8}{\sqrt{2\times 2\times 3}} + \frac{17\times 2^{n+1}-6}{\sqrt{2\times 3\times 2}} + \frac{5\times 2^{n+1}-2}{\sqrt{3\times 2\times 3}} + \frac{7\times 2^{n+2}+20}{\sqrt{2\times 3\times 3}} + \frac{11\times 2^{n+1}+4}{\sqrt{3\times 3\times 3}}.$$

After simplification, we get

$$^2\chi(D_1[n]) = 2^n\left(\frac{28\sqrt{2}}{3} + \frac{115\sqrt{3}}{9}\right) + \frac{15\sqrt{2}}{4} + \frac{7\sqrt{3}}{9},$$

Which proves the theorem.

Theorem 2. The 2-order sum-connectivity index of $D_1[n]$ is calculated as:

$$^2X(D_1[n]) = 2^n\left(2\sqrt{6} + \frac{19\sqrt{2}}{2} + \frac{62\sqrt{7}}{7} + \frac{22}{3}\right) + \frac{9\sqrt{2}+\sqrt{6}}{2} + \frac{4}{3} + \frac{2\sqrt{7}}{7}.$$

Proof. The edge partition of $D_1[n]$is given in Table 1. Now we apply the formula of ^2Xindex to compute this index for$D_1[n]$.Since

$$^2X(D_1[n]) = \sum_{i_1 i_2 i_3} \frac{1}{\sqrt{d_{i_1} + d_{i_2} + d_{i_3}}},$$

Then

$$^2X(D_1[n]) = \frac{3\times 2^{n+2}+3}{\sqrt{2+2+2}} + \frac{7\times 2^{n+2}+8}{\sqrt{2+2+3}} + \frac{17\times 2^{n+1}-6}{\sqrt{2+3+2}} + \frac{5\times 2^{n+1}-2}{\sqrt{3+2+3}}$$

$$+\frac{7\times 2^{n+2}+20}{\sqrt{2+3+3}}+\frac{11\times 2^{n+1}+4}{\sqrt{3+3+3}}.$$

After simplification, we get

$$^{2}X(D_1[n]) = 2^n\left(2\sqrt{6}+\frac{19\sqrt{2}}{2}+\frac{62\sqrt{7}}{7}+\frac{22}{3}\right)+\frac{9\sqrt{2}+\sqrt{6}}{2}+\frac{4}{3}+\frac{2\sqrt{7}}{7},$$

which proves the theorem.

Example 3. We computed the2-order connectivity and 2-order sum-connectivity indices of$D_1[n]$ for various values of n and some results are shown in Table 2.

Table 2: Topological indices of $D_1[n]$

n	$^{2}\chi(D_1[n])$	$^{2}X(D_1[n])$
1	7.731262528917732e + 01	1.078802461574547e + 02
2	1.479747990913464e + 02	2.060825241334871e + 02
3	2.892991466956846e + 02	4.024870800855517e + 02
4	5.719478419043609e + 02	7.952961919896812e + 02
5	1.137245232321714e + 03	1.580914415797940e + 03
6	2.267840013156419e + 03	3.152150863414458e + 03
7	4.529029574825830e + 03	6.294623758647494e + 03
8	9.051408698164651e + 03	1.257956954911357e + 04
9	1.809616694484229e + 04	2.514946113004571e + 04
10	3.618568343819757e + 04	5.028924429190999e + 04

Results for second type of dendrimer

Consider the molecular graph of dendrimer containing viologen-like moiety at the core and naphthalene units at the periphery$D_2[n]$depicted in Figure 3. It is easy to see that the vertex and edge cardinalities are $|V(D_2[n])| = 5\times 2^{n+3}-6$ and$|E(D_2[n])| = 23\times 2^{n+1}-7$ respectively.

Figure 3:Dendrimer containing viologen-like moiety at the core and naphthalene units at the periphery$D_2[n]$ for $n = 1$

Theorem 4. The 2-order connectivity index of $D_2[n]$ is equal to:

$$^{2}\chi(D_2[n]) = \frac{1}{3}\left(2^n(11\sqrt{2}+22\sqrt{3})-5\sqrt{3}\right).$$

Proof. We are ready to compute the 2-order connectivity index of dendrimer$D_2[n]$.To do this,by using Figures 3 and 4, we can fill the Table 3.

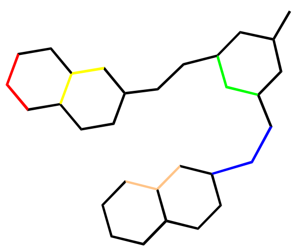

Figure 4: Examples of 2-edges paths of a particular of $D_2[n]$

Table 3: Categorization all 2-edges paths on based their first and end point and the number of these path

$\mathbf{2}$-edges paths	$D_2[1]$	$D_2[2]$	$D_2[3]$	...	$D_2[n]$
$(2,2,2)$	8	16	32	...	2^{n+2}
$(2,2,3)$	32	64	128	...	2^{n+4}
$(2,3,2)$	46	102	214	...	$7\times 2^{n+2}-10$
$(3,2,3)$	12	28	60	...	$2^{n+3}-4$
$(2,3,3)$	20	36	68	...	$2^{n+3}+4$

Since

$$^{2}\chi(D_2[n]) = \sum_{i_1 i_2 i_3} \frac{1}{\sqrt{d_{i_1} d_{i_2} d_{i_3}}},$$

This gives that

$$^{2}\chi(D_2[n]) = \frac{2^{n+2}}{\sqrt{2\times 2\times 2}} + \frac{2^{n+4}}{\sqrt{2\times 2\times 3}} + \frac{7\times 2^{n+2}-10}{\sqrt{2\times 3\times 2}} + \frac{2^{n+3}-4}{\sqrt{3\times 2\times 3}} + \frac{2^{n+3}+4}{\sqrt{2\times 3\times 3}}.$$

After a bit calculation, we get

$$^{2}\chi(D_2[n]) = \frac{1}{3}\left(2^n(11\sqrt{2}+22\sqrt{3}) - 5\sqrt{3}\right),$$

Proving our theorem.

Theorem 5. The 2-order sum-connectivity index of $D_2[n]$ is equal to:

$$^{2}X(D_2[n]) = 2^n\left(4\sqrt{2} + \frac{2\sqrt{6}}{3} + \frac{44\sqrt{7}}{7}\right) - \frac{10\sqrt{7}}{7}.$$

Proof. The required edge partition to compute ^{2}Xindex is in Table 3.Since

$$^{2}X(D_2[n]) = \sum_{i_1 i_2 i_3} \frac{1}{\sqrt{d_{i_1} + d_{i_2} + d_{i_3}}},$$

This implies that

$$^{2}X(D_2[n]) = \frac{2^{n+2}}{\sqrt{2+2+2}} + \frac{2^{n+4}}{\sqrt{2+2+3}} + \frac{7\times 2^{n+2}-10}{\sqrt{2+3+2}} + \frac{2^{n+3}-4}{\sqrt{3+2+3}} + \frac{2^{n+3}+4}{\sqrt{2+3+3}}.$$

After an easy calculation, we get

$$^{2}X(D_2[n]) = 2^n\left(4\sqrt{2} + \frac{2\sqrt{6}}{3} + \frac{44\sqrt{7}}{7}\right) - \frac{10\sqrt{7}}{7},$$

Proving our theorem.

Example 6. We computed the 2-order connectivity and 2-order sum-connectivity indices of $D_2[n]$ for various values of n and some results are shown in Table 4.

Table 4: Topological indices of $D_2[n]$

n	$^2\chi(D_2[n])$	$^2X(D_2[n])$
1	3.288755995579810e + 01	4.406092371741539e + 01
2	6.866187125754433e + 01	9.190149216492306e + 01
3	1.402104938610368e + 02	1.875826290599384e + 02
4	2.833077390680217e + 02	3.789449028499690e + 02
5	5.695022294819916e + 02	7.616694504300303e + 02
6	1.141891210309931e + 03	1.527118545590153e + 03
7	2.286669171965811e + 03	3.058016735910398e + 03
8	4.576225095277569e + 03	6.119813116550889e + 03
9	9.155336941901087e + 03	1.224340587783187e + 04
10	1.831356063514812e + 04	2.449059140039383e + 04

Results for third type of dendrimer

Consider the molecular graph of Naphthyl-decorated dendrimer with cyclam core unit $D_2[n]$ depicted in Figure 5. The vertex and edge cardinalities are $|V(D_3[n])| = 5 \times 2^{n+4} - 22$ and$|E(D_3[n])| = 23 \times 2^{n+2} - 26$ respectively.

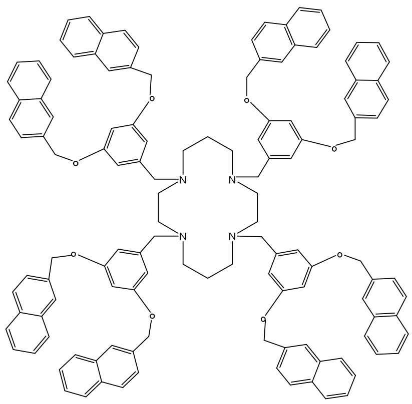

Figure 5: Naphthyl-decorated dendrimer with cyclam core unit$D_3[n]$ for $n = 1$

Theorem 7. The 2-order connectivity index and 2-order sum-connectivity index of $D_3[n]$are computed as:

$$^2\chi(D_3[n]) = \frac{2^n(22\sqrt{2} + 44\sqrt{3}) - 16\sqrt{3}}{3} - \frac{5\sqrt{2}}{6},$$

$$^2X(D_3[n]) = 2^n\left(8\sqrt{2} + \frac{4\sqrt{6}}{3} + \frac{88\sqrt{7}}{7}\right) - 2\sqrt{2} - \frac{32\sqrt{7}}{7} + \frac{\sqrt{6}}{3}.$$

Proof. By considering the general form of this third dendrimer, we can fill the Table 5. These results are proven like pervious theorems therefore, we omit the proofs.

Table 5: Categorization all 2-edges paths on based their first and end point and the number of these path

2-edges paths	$D_3[1]$	$D_3[2]$	$D_3[3]$	...	$D_3[n]$
$(2, 2, 2)$	18	34	66	...	$2^{n+3} + 2$
$(2, 2, 3)$	56	120	248	...	$2^{n+5} - 8$
$(2, 3, 2)$	88	200	424	...	$7 \times 2^{n+3} - 24$
$(3, 2, 3)$	24	56	120	...	$2^{n+4} - 8$
$(2, 3, 3)$	32	64	128	...	2^{n+4}

Example 8. We computed the 2-order connectivity and 2-order sum-connectivity indices of $D_3[n]$ for various values of n and some results are shown in Table 6.

Table 6:Topological indices of $D_3[n]$

n	$^2\chi(D_3[n])$	$^2X(D_3[n])$
1	6.113250699448088e + 01	8.157434321490159e + 01
2	1.326811295979733e + 02	1.772554801099169e + 02
3	2.757783748049583e + 02	3.686177538999476e + 02
4	5.619728652189282e + 02	7.513423014800088e + 02
5	1.134361846046868e + 03	1.516791396640132e + 03
6	2.279139807702747e + 03	3.047689586960377e + 03
7	4.568695731014506e + 03	6.109485967600867e + 03
8	9.147807577638025e + 03	1.223307872888185e + 04
9	1.830603127088506e + 04	2.448026425144381e + 04
10	3.662247865737913e + 04	4.897463529656774e + 04

CONCLUSION

Among topological indices, connectivity indices are very important and they have a prominent role in chemistry. In this paper, the exact expressions for the two connectivity indices termed as 2-order connectivity index and 2-order sum-connectivity index of three types of dendrimers were computed for the first time.

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