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COMPUTING SANSKRUTI INDEX OF DENDRIMER NANOSTARS

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Abstract: Let $G = (V; E)$ be a simple connected graph. The Sanskruti index was introduced by Hosamani [7] and defined as $S(G) = \sum_{uv\in E(G)}(\frac{S_uS_v}{S_u+S_v-2})^3$ where S_u is the summation of degrees of all neighbors of vertex u in G. In this paper, we give explicit formulas for the Sanskruti index of an infinite class of dendrimer nanostars.

Key Words: molecular graph, nanostar dendrimers, Sanskruti index

1. Introduction and Preliminaries

Let $G = (V; E)$ be a simple connected graph. In chemical graph theory, the

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sets of vertices and edges of G are denoted by $V = V(G)$ and $E = E(G)$, respectively. A molecular graph is a simple finite graph such that its vertices correspond to the atoms and the edges to the bonds. A general reference for the notation in graph theory is [1]-[5].

In chemical graph theory, we have many different topological index of arbitrary molecular graph G. A topological index of a graph is a number related to a graph which is invariant under graph automorphisms. Obviously, every topological index defines a counting polynomial and vice versa.

Among topological descriptors, connectivity indices are very important and they have a prominent role in chemistry. One of the best known and widely used is the connectivity index $R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}$introduced in 1975 by Milan Randić (see [6]), who has shown this index to reflect molecular branching.

The Sanskruti index $S(G)$ of a graph G is defined as follows (see [7]):

$$S(G) = \sum_{uv\in E(G)} \left(\frac{S_u S_v}{S_u + S_v - 2}\right)^3 .$$

where S_u is the summation of degrees of all neighbors of vertex u in G. In this paper, we shall give explicit computing formulas for the Sanskruti index of an infinite class of Nanostars Dendrimer $D_3[n]$. For further study, we encourage the reader to consult papers [9]-[26]. In this paper, for every infinite integer n $D_3[n]$ denotes the n^{th} growth of nanostar dendrimer. In following figures, a kind of 3^{th} growth of dendrimer and $D_3[0]$ are shown. Here our notations are standard and mainly taken from standard books of chemical graph theory [1]-[5].

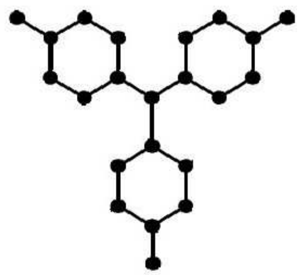

Figure 1: $D_3[0]$ is the primal structure of $D_3[n]$ [17].

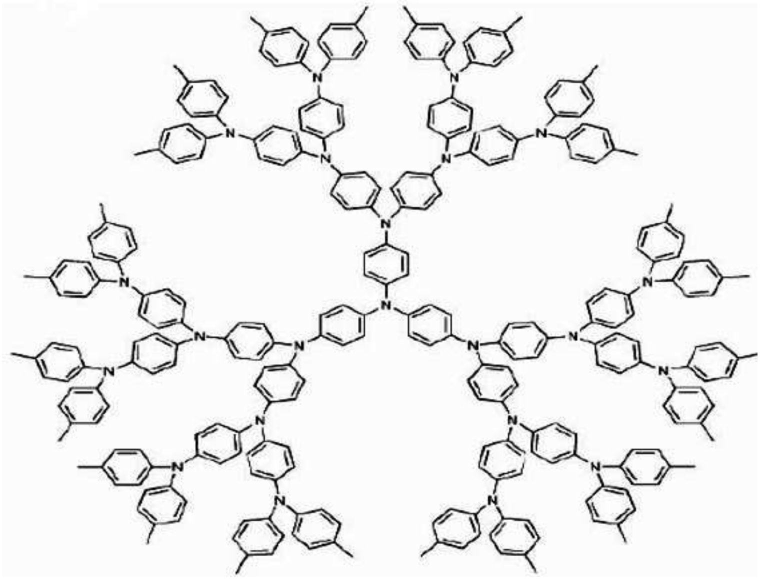

Figure 2: A kind of 3^{th} growth of dendrimer nanostars $D_3[3]$ [17].

2. Main Results and Discussion

Let $D_3[n]$ denote a kind of dendrimer nanostars with n growth stages, see for example Figures 1 and 2, the goal of this paper is to compute a closed formula of this new Connectivity index "Sanskruti index" of $D_3[n]$ for every $n \geq 0$ as follows:

Theorem 2.1. *The Sanskruti index $S(G)$ of Nanostar Dendrimer $D_3[n]$ for every $n \geq 0$ is equal to*

$$S(D_3[n]) = \frac{338061}{512}2^n + \frac{60875}{192}2^{n+1} - \frac{135107}{144} + \frac{250047}{4096}3^{2n}.$$

Proof. Consider Nanostar Dendrimer $D_3[n]$ for every $n \geq 0$, (see Figures 1 and 2). From Figure 2 and Ref. [17], one can see that the number of vertices/atoms in this nanostar is equal to $|V(D_3[n])| = 24(2^n) - 20$ and also the number of edges/bonds is $|E(D_3[n])| = 24(2^{n+1} - 1)$.

Since all vertices/atoms of nanostar Dendrimer have degree $3, 2$ and 1 (hydrogen (H) atom), we divide the vertex/atom set of $D_3[n]$ in three partitions as

$$V_3 = \{v \in V(D_3[n]) | d_v = 3\},$$

$$V_2 = \{v \in V(D_3[n]) | d_v = 2\}, \text{ and}$$
$$V_1 = \{v \in V(D_3[n]) | d_v = 1\}.$$

By according to the 2−Dimensional of dendrimer $D_3[n]$ in Figure 2, one can see that

$$|V_1[n]| = 3(2^n),$$
$$|V_2[n]| = 12(2^{n+1} - 1),$$
$$|V_3[n]| = 15(2^n) - 8.$$

New we can divide the edge/bond set $E(D_3[n])$ in three partitions as follow:

$$E_6 = \{u, v \in V(D_3[n]) | d_u = d_v = 3\}$$
$$E_5 = \{u, v \in V(D_3[n]) | d_u = 3 \text{ and } d_v = 2\},$$
$$E_4 = \{u, v \in V(D_3[n]) | d_u = d_v = 2 \text{ or } d_u = 3 \text{ and } d_v = 1\}.$$

From Figure 2 one can see that $|E_4| = 15(2^n) - 6$, $|E_5| = 12(2^{n+1} - 1)$ and $|E_6| = 9(2^n) - 6$.

And also, summation of degrees of edge endpoints of this nanostar have six types $e_{(3,5)}$, $e_{(5,5)}$, $e'_{(5,5)}$,$e_{(5,7)}$, $e_{(7,9)}$ and $e_{(9,9)}$ that are shown in Figure 2 by red, yellow, green, blue, hoary and black colors. Since for all edge $e = uv$ of the types $e_{(3,5)}$, $S_v = 3$ (for all hydrogen H atom) and $S_u = 5$ and for an edge xy of the types $e'_{(5,5)}$, $S_x = S_y = 5$, such that vertices x and y are one of adjacent vertices of degree 2 and other types are analogous. From Figure 2, the number of edges of these edge types are shown in following table.

Summation of degrees of edge endpoints	$e_{(3,5)}$)	$e_{(5,5)}$	$e'_{(5,5)}$	$e_{(5,7)}$	$e_{(7,9)}$	and $e_{(9,9)}$
Number of edges of this type	$3(2^n)$	$6(2^n)$	$6(2^{n+1} - 1)$	$9(2^{n+1}) - 12$	$3(2^n)$	$6(2^n - 1)$

Thus, by using above Table and Figure 3, we can deduce the following formula for Sanskruti index $S(G)$ of Nanostar Dendrimer $D_3[n]$ $\forall n \geq 0$, as follow:

$$S(D_3[n]) = \sum_{uv \in E(G)} \left(\frac{S_u S_v}{S_u + S_v - 2} \right)^3$$
$$= \frac{338061}{512} 2^n + \frac{60875}{192} 2^{n+1} - \frac{135107}{144} + \frac{250047}{4096} 3^{2n}. \qquad \square$$

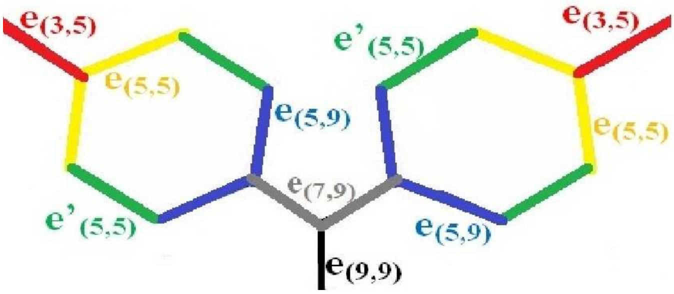

Figure 3: Six edge types of Nanostar Dendrimer $D_3[n]$ [23].

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