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Atom Bound Connectivity, Zagreb, Sombor, Nirmala and Harmonic Indices of Dendrimers

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Abstract

A nanostar is a very small molecule ranging in size from 1-100 nanometers. It is typically composed of materials such as polymers, silica and others. Nanostars are of great significance in various fields, including drug technology, energy technology and other applications. The topological index is a numerical depiction of a molecular structure. Within chemical graphs, the atoms and the chemical bonds connecting them are symbolized by vertices and edges, respectively. Topological indices help to predict the topological properties of nanostar dendrimers, such as molecular weight and size. In this article, we computed the first Zagreb index, the second Zagreb Index, the third Zagreb index, Sombor index, ABC index, Nirmala index and Harmonic index of two new families of nanostar dendrimers such as NS_1 is also known as aminoisophthalate diester monomer and PD_1 known as Poly (amidoamine).

Introduction:

Let G be a simple and connected graph with set of vertex V(G) and set of edges S(G). The degree of a vertex t is the number of vertices adjacent to t and it is denoted by d_t. A molecular graph is a graph where the vertices represent atoms and the edges represent bonds between them. Chemical graph theory is a branch of Mathematical Chemistry that focuses on finding topological indices of a molecular graph that correlate well with chemical properties of the chemical molecules '[1]'.

Topological indices are very important numerical paramrters that help to determine the physical and biological properties in organic compounds. For example, the Nirmala and ABC indices help determine the degree of acidity and characterize the structure of the molecule in compounds. As for the harmonic index, the study of which ia an active area in chemical research, as it is related to the electronic energy of some molecules.

Mohamad.N.Husin et.al. investigated Zagreb polynomial for several dendrimeres such as PAMAM dendrimers and tetrathiafulvalene dendrimer '([2]'. Additionaly, Muhammad.K.siddiqui et.al. calculated the Zagreb indices for some nanostar dindrimers such as polyphenylene dendrimer '[3]'.

And Shin.M.Kang et.al. are computed redefine 1^{st}, 2^{nd} and 3^{rd} Zagreb indices of nanostar dendrimers such as polypropylenimine octaamin ([4]).

Therefor, the equation for the 1st Zagreb polynomial, 2nd Zagreb polynomial and 3rd Zagreb indices of graph G is defined as' [4][3]':

$$\mathbf{M_1(G) = \sum_{ut\in S(G)} d_u + d_t}$$
$$\mathbf{M_2(G) = \sum_{ut\in S(G)} d_u \times d_t}$$
$$\mathbf{M_3(G) = \sum_{ut\in S(G)} |d_u - d_t|}$$

Kinkar Ch.Das et.al. are presented novel lower and upper bounds on the Sombor index of graphs by using some graph parameters and they obtained several relations on Sombor index with the first and second Zagreb indices of graphs([5]). And Roberto Cruz et.al. are studed sombor index on chemical graph([6]). Ammar Alsinai et.Al. are tested the sombor index with physico-chemical properties of octane isomers such as entropy, acentric factor enthalpy of vaporization (HVAP) and standard enthalpy of vaporization (DHVAP) using the linear models. The Sombor index shows excellen correlation with these chemical properties.Further, they optained Sombor index of 2D-lattice, nanotube and nanotorus of TUC_4C_8[p,q] and subdivision graph of 2D-lattice nanotube and nanotorus of TUC_4C_8[p,q] '[7]'.

The Sombor index of graph G is defined as '[8]':

$$SO(G) = \sum_{ut\in S(G)} \sqrt{(d_u)^2 + (d_t)^2}$$

S.Alikhani et.al. are computed the ABC index for some families of nanostar and polyphenylene dendrimer ([9]). And Kinkar Ch.Das is presented the lower and upper bounds on index of graphs and trees, and charac-
terize graphs for which these bounds are best possible '[10]'. Mohamad.N.Husin et.al. Are studied the fourth version of ABC index and the fifth version of GA index of some families of nanostar dendrimers '[11]'.

The ABC index of graph G is defined as '[11]' :

$$ABC(G) = \sum_{ut\in S(G)} \sqrt{\frac{d_u+d_t-2}{d_u d_t}}$$

V.R.Kulli examined Nirmala polynomial of various dendrimers such as porphyrin dedrimers , propyl ether imine dendrimer and Poly ethylene amide amine Dendrimer '[12]'. Additionally V.R.Kulli et.al. caclculated Nirmala index for different chemical networks including silicate networks, chain silicate networks, hexagona networks, oxide networks and honeycomb networks' [13]'.

The Nirmala index of graph G is defined as '[12][13]':

$$N(G) = \sum_{ut\in S(G)} \sqrt{d_u + d_t}$$

Muhammad.K.Jamil et.al. Computed the harmonic polynomial and harmonic index of some nanotubes like TUC_4C_8[m,n] and $TUC_4[m, n]$ '[14]'.
Juan.C.Hern ́andez-Gomez et.al. Are studed harmonic index and harmonic polynomial of several classical symmetric operations of graphs '[15]'.

The harmonic polynomial of a graph G is defined as '[14]':

$$H(G) = \sum_{ut\in S(G)} \frac{2}{d_u+d_t}$$

in this paper we compyted 1st Zagreb indexl, 2nd Zagreb index, 3rd Zagreb index, sombor index, ABC index. Nirmala index and harmonic index of a number of type nanostar dendrimers like NS_1 is also known as aminoisophthalate diester monomer and PD_1 is also known as Poly (amidoamine).

1) first kind of nanostar dendrimer NS_1: we consider the first kind nanostar dendrimer $NS_1[n]$ the order of $NS_1[n]$ is $30\times 2^{n+1}-48$ and the size of $NS_1[n]$ is $33\times 2^{n+1}-54$. Figure 1.Shwos**.**

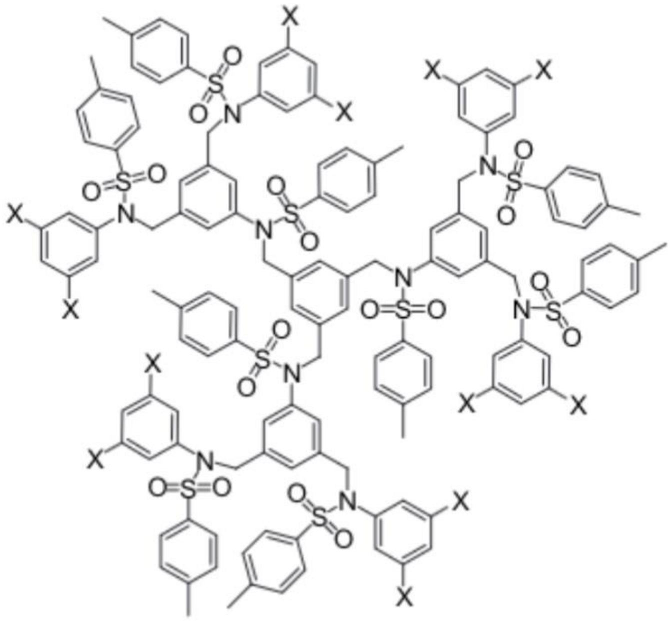

Fig.1. Nanostar dendrimers $NS_1[n]$ is also known as aminoisophthalate diester monomer

In $NS_1[n]$ there is six several kinds of edges as given in **table 1.**

Table 1. The molecular graph of $NS_1[n]$

(d_t, d_u)	(1,2)	(1,3)	(1,4)	(2,2)	(2,3)	(3,4)
No. Of edges	3×2^n	$3\times 2^n-3$	$6\times 2^n-6$	$6\times 2^n-6$	$42\times 2^n-33$	$6\times 2^n-6$

Theorem1.1*:* let n∈ N s.t n={ 0,1,2,3....} then 1st Zagreb indexl, 2nd Zagreb index, 3rd Zagreb index is of NS_1 is given as:

$$M_1(NS_1[n]) = 327\times 2^n-273$$

$$M_2(NS_1[n]) = 387\times 2^n-327$$

$$M_3(NS_1[n]) = 76\times 2^n-63$$

Proof: : the edge set of nanostar dendrimers NS_1 is partitioned into six set, S_1 consists3×2^n edges of type u-t s.t. $d_u=1$, $d_t=2$, S_2 consists $3\times 2^n-3$ edges of type u-t s.t. $d_u=1$, $d_t=3$, S_3 consists $6\times 2^n-6$ edges of kind u-t s.t. $d_u=1$, $d_t=4$, S_4 consists $6\times 2^n-6$ edges of kind u-t s.t. $d_u=2$, $d_t=2$, S_5 consists $42\times 2^n-33$ edges of kind u-t s.t. $d_u=2$, $d_t=3$ and S_6 consists $6\times 2^n-6$ edges of kind u-t s.t. $d_u=3$, $d_t=4$.

$$Z_1(NS_1[n],X) = (6\times 2^n-6)X^7+(48\times 2^n-39)X^5+(9\times 2^n-9)X^4+(3\times 2^n)X^3$$

$$\frac{d}{dx}[Z_1(NS_1[n],X)]_{x=1} = (42\times 2^n - 42) + (240\times 2^n - 195) + (36\times 2^n - 36) + (9\times 2^n)$$

$$= 327 \times 2^n - 273$$

$$= \sum_{ut\in S(G)} d_u + d_t$$

$$\frac{d}{dx}[Z_1(NS_1[n],X)]_{x=1} = M_1(NS_1[n])$$

$$Z_2(NS_1[n],X) = (6\times 2^n - 6)X^{12} + (42\times 2^n - 33)X^6 + (12\times 2^n - 12)X^4 + (3\times 2^n - 3)X^3 + (3\times 2^n)X^2$$

$$\frac{d}{dx}[Z_2(NS_1[n],X)]_{x=1} = (72\times 2^n - 72) + (252\times 2^n - 198) + (48\times 2^n - 48) + (9\times 2^n - 9) + (96\times 2^n)$$

$$= 387 \times 2^n - 327$$

$$= \sum_{ut\in S(G)} d_u \times d_t$$

$$\frac{d}{dx}[Z_2(NS_1[n],X)]_{x=1} = M_2(NS_1[n])$$

$$Z_3(NS_1[n],X) = (6\times 2^n - 6)X^3 + (3\times 2^n - 3)X^2 + (51\times 2^n - 39)X + (3\times 2^n)$$

$$\frac{d}{dx}[Z_3(NS_1[n],X)]_{x=1} = (18\times 2^n - 18) + (6\times 2^n - 6) + (51\times 2^n - 39)$$

$$= (76\times 2^n - 63)$$

$$= \sum_{ut\in S(G)} |d_u - d_t|$$

$$\frac{d}{dx}[Z_3(NS_1[n],X)]_{x=1} = M_3(NS_1[n])$$

Theorem1.2: let n∈ N s.t n≥ 0 then the sombor index of NS_1 is given as :

$$SO(NS_1[n]) = (48\sqrt{13} + 12\sqrt{2} + 3\sqrt{10} + 3\sqrt{5} + 30\times 2^n) - (33\sqrt{13} + 6\sqrt{17} + 3\sqrt{10} + 12\sqrt{2} + 30)$$

Proof: : the edge set of nanostar dendrimers NS_1 is partitioned into six set, S_1 consists 3×2^n edges of type u-t s.t. $d_u = 1$, $d_t = 2$, S_2 consists $3\times 2^n - 3$ edges of type u-t s.t. $d_u = 1$, $d_t = 3$, S_3 consists $6\times 2^n - 6$ edges of kind u-t s.t. $d_u = 1$, $d_t = 4$, S_4 consists $6\times 2^n - 6$ edges of kind u-t s.t. $d_u = 2$, $d_t = 2$, S_5 consists $42 \times 2^n - 33$ edges of kind u-t s.t. $d_u = 2$, $d_t = 3$ and S_6 consists $6 \times 2^n - 6$ edges of kind u-t s.t. $d_u = 3$, $d_t = 4$.

$$SO(NS_1[n]) = \sum_{ut\in S1}\sqrt{(d_u)^2 + (d_t)^2} + \sum_{ut\in S2}\sqrt{(d_u)^2 + (d_t)^2} + \sum_{ut\in S3}\sqrt{(d_u)^2 + (d_t)^2} + \sum_{ut\in S4}\sqrt{(d_u)^2 + (d_t)^2}$$

$$+ \sum_{ut\in S5}\sqrt{(d_u)^2 + (d_t)^2} + \sum_{ut\in S6}\sqrt{(d_u)^2 + (d_t)^2}$$

$$= (3\times 2^n)\sqrt{(1)^2 + (2)^2} + (3\times 2^n - 3)\sqrt{(1)^2 + (3)^2} + (6\times 2^n - 6)\sqrt{(1)^2 + (4)^2} + (6\times 2^n - 6)\sqrt{(2)^2 + (2)^2}$$

$$+ (42\times 2^n - 33)\sqrt{(2)^2 + (3)^2} + (6\times 2^n - 6)\sqrt{(3)^2 + (4)^2}$$

$$= (3\sqrt{5} \times 2^n) + (3\sqrt{10} \times 2^n - 3\sqrt{10}) + (6\sqrt{17} \times 2^n - 6\sqrt{17}) + (12\sqrt{2} \times 2^n - 12\sqrt{2}) + (42\sqrt{13} \times 2^n - 33\sqrt{13})$$

$$+ (30\times 2^n - 30)$$

$$= (48\sqrt{13} + 12\sqrt{2} + 3\sqrt{10} + 3\sqrt{5} + 30 \times 2^n) - (33\sqrt{13} + 6\sqrt{17} + 3\sqrt{10} + 12\sqrt{2} + 30)$$

Theorem1.3*:* let n$\in$ N s.t n≥ 0 then the atom bound connectivety of NS_1 is given as :

$$ABC(NS_1[n]) = (\frac{51\sqrt{2}}{2} + \sqrt{6} + 3\sqrt{3} + \frac{\sqrt{15}}{3} \times 2^n) - (\frac{39\sqrt{2}}{2} + 3\sqrt{3} + \sqrt{6} + \frac{\sqrt{15}}{3})$$

Proof: : the edge set of nanostar dendrimers NS_1 is partitioned into six set, S_1 consists 3×2^n edges of type u-t s.t. $d_u = 1$, $d_t = 2$, S_2 consists $3 \times 2^n - 3$ edges of type u-t s.t. $d_u = 1$, $d_t = 3$, S_3 consists $6 \times 2^n - 6$ edges of kind u-t s.t. $d_u = 1$, $d_t = 4$, S_4 consists $6 \times 2^n - 6$ edges of kind u-t s.t. $d_u = 2$, $d_t = 2$, S_5 consists $42 \times 2^n - 33$ edges of kind u-t s.t. $d_u = 2$, $d_t = 3$ and S_6 consists $6 \times 2^n - 6$ edges of kind u-t s.t. $d_u = 3$, $d_t = 4$.

$$ABC(NS_1[n]) = \sum_{ut\in S1}\sqrt{\frac{d_u+d_t-2}{d_u d_t}} + \sum_{ut\in S2}\sqrt{\frac{d_u+d_t-2}{d_u d_t}} + \sum_{ut\in S3}\sqrt{\frac{d_u+d_t-2}{d_u d_t}} + \sum_{ut\in S4}\sqrt{\frac{d_u+d_t-2}{d_u d_t}} +$$

$$\sum_{ut\in S5}\sqrt{\frac{d_u+d_t-2}{d_u d_t}} + \sum_{ut\in S6}\sqrt{\frac{d_u+d_t-2}{d_u d_t}}$$

$$= (3\times 2^n)\sqrt{\frac{1+2-2}{1\times 2}} + (3\times 2^n - 3)\sqrt{\frac{1+3-2}{1\times 3}} + (6\times 2^n - 6)\sqrt{\frac{1+4-2}{1\times 4}} + (6\times 2^n - 6)\sqrt{\frac{2+2-2}{2\times 2}} + (42\times 2^n - 33)\sqrt{\frac{2+3-2}{2\times 3}} + (6\times 2^n - 6)\sqrt{\frac{3+4-2}{3\times 4}}$$

$$= (\frac{3\sqrt{2}}{2}\times 2^n) + (\sqrt{6}\times 2^n - \sqrt{6}) + (3\sqrt{3}\times 2^n - 3\sqrt{3}) + (3\sqrt{2}\times 2^n - 3\sqrt{2}) + (21\sqrt{2}\times 2^n - \frac{33\sqrt{2}}{2}) + (\frac{\sqrt{15}}{3}\times 2^n - \frac{\sqrt{15}}{3})$$

$$= (\frac{51\sqrt{2}}{2} + \sqrt{6} + 3\sqrt{3} + \frac{\sqrt{15}}{3}\times 2^n) - (\frac{39\sqrt{2}}{2} + 3\sqrt{3} + \sqrt{6} + \frac{\sqrt{15}}{3})$$

Theorem 1.4: Consider n∈ N s.t n≥ 0 then the nirmala index of of NS_1 is given as :

$$N(NS_1[n]) = (48\sqrt{5} + 18 + 6\sqrt{7} + 3\sqrt{3}\times 2^n) - (39\sqrt{5} + 18 + 6\sqrt{7})$$

Proof: : the edge set of nanostar dendrimers NS_1 is partitioned into six set, S_1 consists 3×2^n edges of type u-t s.t. $d_u = 1$, $d_t = 2$, S_2 consists $3\times 2^n - 3$ edges of type u-t s.t. $d_u = 1$, $d_t = 3$, S_3 consists $6\times 2^n - 6$ edges of kind u-t s.t. $d_u = 1$, $d_t = 4$, S_4 consists $6\times 2^n - 6$ edges of kind u-t s.t. $d_u = 2$, $d_t = 2$, S_5 consists $42\times 2^n - 33$ edges of kind u-t s.t. $d_u = 2$, $d_t = 3$ and S_6 consists $6\times 2^n - 6$ edges of kind u-t s.t. $d_u = 3$, $d_t = 4$.

$$N(NS_1[n]) = N(G) = \sum_{ut\in S1}\sqrt{d_u + d_t} + \sum_{ut\in S2}\sqrt{d_u + d_t} + \sum_{ut\in S3}\sqrt{d_u + d_t} + \sum_{ut\in S4}\sqrt{d_u + d_t} + \sum_{ut\in S5}\sqrt{d_u + d_t} + \sum_{ut\in S6}\sqrt{d_u + d_t}$$

$$= (3\times 2^n)\sqrt{1+2} + (3\times 2^n - 3)\sqrt{1+3} + (6\times 2^n - 6)\sqrt{1+4} + (6\times 2^n - 6)\sqrt{2+2} + (42\times 2^n - 33)\sqrt{2+3} + (6\times 2^n - 6)\sqrt{3+4}$$

$$= (3\sqrt{3}\times 2^n) + (6\times 2^n - 6) + (6\sqrt{5}\times 2^n - 6\sqrt{5}) + (12\times 2^n - 12) + (42\sqrt{5}\times 2^n - 33\sqrt{5}) + (6\sqrt{7}\times 2^n - 6\sqrt{7})$$

$$= (48\sqrt{5} + 18 + 6\sqrt{7} + 3\sqrt{3}\times 2^n) - (39\sqrt{5} + 18 + 6\sqrt{7})$$

Theorem1.5: : Consider n∈ N s.t n≥ 0 then the harmonic index of of NS_1 is given as :

$$H(NS_1[n]) = \frac{1919}{70}\times 2^n - \frac{1527}{70}$$

Proof: : the edge set of nanostar dendrimers NS_1 is partitioned into six set, S_1 consists 3×2^n edges of type u-t s.t. $d_u = 1$, $d_t = 2$, S_2 consists $3\times 2^n - 3$ edges of type u-t s.t. $d_u = 1$, $d_t = 3$, S_3 consists $6\times 2^n - 6$ edges of kind u-t s.t. $d_u = 1$, $d_t = 4$, S_4 consists $6\times 2^n - 6$ edges of kind u-t s.t. $d_u = 2$, $d_t = 2$, S_5 consists $42 \times 2^n - 33$ edges of kind u-t s.t. $d_u = 2$, $d_t = 3$ and S_6 consists $6 \times 2^n - 6$ edges of kind u-t s.t. $d_u = 3$, $d_t = 4$.

$$H(NS_1[n]) = \sum_{ut\in S1}\frac{2}{d_u+d_t} + \sum_{ut\in S2}\frac{2}{d_u+d_t} + \sum_{ut\in S3}\frac{2}{d_u+d_t} + \sum_{ut\in S4}\frac{2}{d_u+d_t} + \sum_{ut\in S5}\frac{2}{d_u+d_t} + \sum_{ut\in S6}\frac{2}{d_u+d_t}$$

$$= (3\times 2^n)\frac{2}{1+2} + (3\times 2^n - 3)\frac{2}{1+3} + (6\times 2^n - 6)\frac{2}{1+4} + (6\times 2^n - 6)\frac{2}{2+2} + (42\times 2^n - 33)\frac{2}{2+3} + (6\times 2^n - 6)\frac{2}{3+4}$$

$$= (2\times 2^n) + (\frac{3}{2}\times 2^n - \frac{3}{2}) + \left(\frac{12}{5}\times 2^n - \frac{12}{5}\right) + (3\times 2^n - 3) + \left(\frac{84}{5}\times 2^n - \frac{66}{5}\right) + (\frac{12}{7}\times 2^n - \frac{12}{7})$$

$$= \frac{1919}{70}\times 2^n - \frac{1527}{70}$$

***2)** second kind of nanostar dendrimer PD_1*: we consider the first kind nanostar dendrimer $PD_1[n]$ the order of $PD_1[n]$ is $12\times 2^{n+2} - 14$ and the size of $PD_1[n]$ is $12\times 2^{n+2} - 15$. Figure 2. Shows**.**

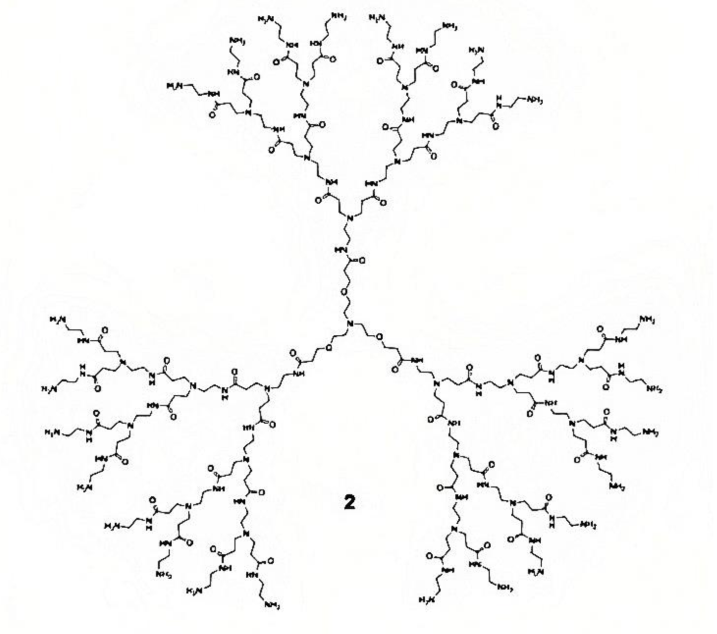

Fig.2. Nanostar dendrimers PD_1 is also known as Poly (amidoamine).

In $PD_1[n]$ there is four several kinds of edges as given in **table 2.**

Table 2. The molecular graph of PD_1 [n]

(d_t, d_u)	(1,2)	(1,3)	(2,2)	(2,3)
No. Of edges	3×2^n	$6\times 2^n - 3$	18×2^n	$21\times 2^n - 12$

Theorem2.2: : let n∈ N s.t n={ 0,1,2,3....} then 1^{st} Zagreb indexl, 2^{nd} Zagreb index, 3^{rd} Zagreb index is of PD_1 is given as:

$$M_1(PD_1[n]) = 210 \times 2^n - 72$$

$$M_2(PD_1[n]) = 222 \times 2^n - 81$$

$$M_3(PD_1[n]) = 36 \times 2^n - 18$$

Proof: : the edge set of nanostar dendrimers PD_1 is partitioned into four set, S_1 consists 3×2^n edges of type u-t s.t. $d_u = 1$, $d_t = 2$, S_2 consists $6 \times 2^n - 3$ edges of type u-t s.t. $d_u = 1$, $d_t = 3$, S_3 consists 18×2^n edges of kind u-t s.t. $d_u = 2$, $d_t = 2$, S_5 consists $21 \times 2^n - 12$ edges of kind u-t s.t. $d_u = 2$, $d_t = 3$.

$$Z_1 (PD_1 [n],X) = (21\times 2^n -12) X^5 + (24\times 2^n -3) X^4 + (3\times 2^n) X^3$$

$$\frac{D}{DX}[Z_1 (PD_1[N], X)]_{x=1} = (105\times 2^N - 60) + (96 \times 2^n - 12) + (9 \times 2^N)$$

$$= (210\times 2^n - 72)$$

$$= \sum_{ut\in S(G)} d_u + d_t$$

Thus,

$$\frac{d}{dx}[Z_1 (PD_1[n], X)]_{x=1} = M_1(PD_1[n])$$

$$Z_2 (PD_1 [n],X) = (21\times 2^n -12) X^6 + (18\times 2^n)X^4 + (6\times 2^n -3)X^3 + (3\times 2^n)X^2$$

$$\frac{d}{dx}[Z_2 (PD_1[n], X)]_{x=1} = (126\times 2^n -72) + (72\times 2^n) + (18\times 2^n -9) + (6\times 2^n)$$

$$= (222\times 2^n -81)$$

$$=\sum_{ut\in S(G)} d_u \times d_t$$

Thus,

$$\frac{d}{dx}[Z_2 (PD_1[n], X)]_{x=1} = M_2(PD_1[n])$$

$$Z_3\ (PD_1[n]\ ,X) = (6\times\ 2^n\ \text{-}3)X^2+(24\times\ 2^n\ \text{-}12)X + (18\times\ 2^n)$$

$$\frac{d}{dx}[Z_3\ (PD_1[n],X)]_{\ x=1} = (12\times\ 2^n\ \text{-}6) + (24\times\ 2^n\ \text{-}12)$$

$$= (36\times\ 2^n\ \text{-}18)$$

$$= \sum_{ut\in S(G)} |d_u - d_t|$$

Thus,

$$\frac{d}{dx}[Z_3\ (PD_1[n],X)]_{\ x=1} = M_3(PD_1[n])$$

Theorem2.2: let n∈ N s.t n≥ 0 then the sombor index of PD_1 is given as :

$$SO\ (NS_1[n]) = (21\sqrt{13} + 36\sqrt{2} + 6\sqrt{10} + 3\sqrt{5}\ \times 2^n) - (12\sqrt{13} + 3\sqrt{10}\ )$$

Proof: the edge set of nanostar dendrimers PD_1 is partitioned into four set, S_1 consists 3× 2^n edges of type u-t s.t. $d_u = 1$, $d_t = 2$, S_2 consists $6 \times 2^n - 3$ edges of type u-t s.t. $d_u = 1$, $d_t = 3$, S_3 consists 18×2^n edges of kind u-t s.t. $d_u = 2$, $d_t = 2$, S_5 consists $21 \times 2^n - 12$ edges of kind u-t s.t. $d_u = 2$, $d_t = 3$.

$$SO(PD_1[n]) = \sum_{ut\in S1}\sqrt{(d_u)^2 + (d_t)^2} + \sum_{ut\in S2}\sqrt{(d_u)^2 + (d_t)^2} + \sum_{ut\in S3}\sqrt{(d_u)^2 + (d_t)^2} +$$

$$\sum_{ut\in S4}\sqrt{(d_u)^2 + (d_t)^2}$$

$$= (3\times 2^n)\sqrt{(1)^2 + (2)^2} + (6\times 2^n - 3)\sqrt{(1)^2 + (3)^2} + (18\times 2^n)\sqrt{(2)^2 + (2)^2} + (21\times 2^n -$$

$$12)\sqrt{(2)^2 + (3)^2}$$

$$= (3\sqrt{5} \times 2^n) + (6\sqrt{10} \times 2^n - 3\sqrt{10}) + (36\sqrt{2} \times 2^n) + (12\sqrt{13} \times 2^n - 12\sqrt{13})$$

$$= (21\sqrt{13} + 36\sqrt{2} + 6\sqrt{10} + 3\sqrt{5}\ \times 2^n) - (12\sqrt{13} + 3\sqrt{10}\ )$$

Theorem2.3: let n∈ N s.t n≥ 0 then the atom bound connectivety of PD_1 is given as :

$$ABC(PD_1[n]) = (\ 21\sqrt{2} + 2\sqrt{6}\ \times 2^n) - 7\sqrt{6}$$

Proof: the edge set of nanostar dendrimers PD_1 is partitioned into four set, S_1 consists 3× 2^n edges of type u-t s.t. $d_u = 1$, $d_t = 2$, S_2 consists $6 \times 2^n - 3$ edges of type u-t s.t. $d_u = 1$, $d_t = 3$, S_3 consists 18×2^n edges of kind u-t s.t. $d_u = 2$, $d_t = 2$, S_5 consists $21 \times 2^n - 12$ edges of kind u-t s.t. $d_u = 2$, $d_t = 3$.

$$ABC(PD_1[n]) = \sum_{ut\in S1}\sqrt{\frac{d_u+d_t-2}{d_u d_t}} + \sum_{ut\in S2}\sqrt{\frac{d_u+d_t-2}{d_u d_t}} + \sum_{ut\in S3}\sqrt{\frac{d_u+d_t-2}{d_u d_t}} + \sum_{ut\in S4}\sqrt{\frac{d_u+d_t-2}{d_u d_t}}$$

$$= (3\times 2^{n})\sqrt{\frac{1+2-2}{1\times 2}} + (6\times 2^{n} - 3)\sqrt{\frac{1+3-2}{1\times 3}} + (18\times 2^{n})\sqrt{\frac{2+2-2}{2\times 2}} + (21\times 2^{n} - 12)\sqrt{\frac{2+3-2}{2\times 3}}$$

$$= (\frac{3\sqrt{2}}{2} \times 2^{n}) + \left(2\sqrt{6} \times 2^{n} - \sqrt{6}\right) + (9\sqrt{2} \times 2^{n}) + (\frac{21\sqrt{2}}{2} \times 2^{n} - 6\sqrt{2})$$

$$= (21\sqrt{2} + 2\sqrt{6} \times 2^{n}) - 7\sqrt{6}$$

Theorem 2.4: Consider n∈ N s.t n≥ 0 then the nirmala index of of PD_1 is given as :

$$N(PD_1[n]) = (48 + 21\sqrt{5} + 3\sqrt{3} \times 2^{n}) - (12\sqrt{5} + 6)$$

Proof: the edge set of nanostar dendrimers PD_1 is partitioned into four set, S_1 consists 3×2^n edges of type u-t s.t. $d_u = 1$, $d_t = 2$, S_2 consists $6 \times 2^n - 3$ edges of type u-t s.t. $d_u = 1$, $d_t = 3$, S_3 consists 18×2^n edges of kind u-t s.t. $d_u = 2$, $d_t = 2$, S_5 consists $21 \times 2^n - 12$ edges of kind u-t s.t. $d_u = 2$, $d_t = 3$.

$$N(PD_1[n]) = \sum_{ut\in S1}\sqrt{d_u + d_t} + \sum_{ut\in S2}\sqrt{d_u + d_t} + \sum_{ut\in S3}\sqrt{d_u + d_t} + \sum_{ut\in S4}\sqrt{d_u + d_t}$$

$$= (3\times 2^{n})\sqrt{1+2} + (6\times 2^{n} - 3)\sqrt{1+3} + (18\times 2^{n})\sqrt{2+2} + (21\times 2^{n} - 12)\sqrt{2+3}$$

$$= (3\sqrt{3} \times 2^{n}) + (12\times 2^{n} - 6) + (36\times 2^{n}) + (21\sqrt{5} \times 2^{n} - 12\sqrt{5})$$

$$= (48 + 21\sqrt{5} + 3\sqrt{3} \times 2^{n}) - (12\sqrt{5} + 6)$$

Theorem2.5: : Consider n∈ N s.t n≥ 0 then the harmonic index of of PD_1 is given as :

$$H(PD_1[n]) = \frac{112}{5} \times 2^{n} - \frac{63}{10}$$

Proof: the edge set of nanostar dendrimers PD_1 is partitioned into four set, S_1 consists 3×2^n edges of type u-t s.t. $d_u = 1$, $d_t = 2$, S_2 consists $6 \times 2^n - 3$ edges of type u-t s.t. $d_u = 1$, $d_t = 3$, S_3 consists 18×2^n edges of kind u-t s.t. $d_u = 2$, $d_t = 2$, S_5 consists $21 \times 2^n - 12$ edges of kind u-t s.t. $d_u = 2$, $d_t = 3$.

$$H(PD_1[n]) = \sum_{ut\in S1}\frac{2}{d_u+d_t} + \sum_{ut\in S2}\frac{2}{d_u+d_t} + \sum_{ut\in S3}\frac{2}{d_u+d_t} + \sum_{ut\in S4}\frac{2}{d_u+d_t}$$

$$= (3\times 2^{n})\frac{2}{1+2} + (6\times 2^{n} - 3)\frac{2}{1+3} + (18\times 2^{n})\frac{2}{2+2} + (21\times 2^{n} - 12)\frac{2}{2+3}$$

$$= (2\times 2^{n}) + (3 \times 2^{n} - \frac{3}{2}) + (9 \times 2^{n}) + \left(\frac{42}{5} \times 2^{n} - \frac{24}{5}\right) + (\frac{12}{7} \times 2^{n} - \frac{12}{7})$$

$$= \frac{112}{5} \times 2^{n} - \frac{63}{10}$$

***Conclusion**:* In this study,we seek to contribute to helping researchers to kmow the importance of molecular topology in mathematics and chemistry. Therefore, we calculated two new different infinite families of nanostar dendrimers like NS_1 is also known as aminoisophthalate diester monomer and PD_1 known as Poly (amidoamine) using some topological indices such as (the first Zagreb index, the second Zagreb index, the third Zagreb index, Sombor index, the atom bound connectivity index, Nirmala index and harmonic index).

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مؤشرات اتصال ربط الذرة، زاغرب، سومبور، نيرمالا والتوافقي لبعض المتغصنات

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مؤشر زاغرب، مؤشر سومبور، مؤشر ABC، مؤشر نيرمالا، مؤشر التوافقي، متغصن النانو ستار

معلومات المؤلف

الايميل:

الخلاصة:

النانوستار عبارة عن جزئ صغير للغاية يتراوح حجمه من 1 الى 100 نانومتر. ويتشكل عادة من مواد مثل البوليمرات والسيليكا وغيرها. تعتبر النانوستار ذات اهمية كبيرة في مجالات مختلفة، بما في ذلك تكنولوجيا صناعة الادوية وتكنولوجيا الطاقة وغيرها من التطبيقات. المؤشر الطوبولوجي هو تصوير رقمي للبنية الجزيئية. ضمن الرسوم البيانية الكيميائية، ترمز للذرات والروابط الكيميائية التي تربطها بالرؤوس والحواف، على التوالي. تساعد المؤشرات الطوبولوجية على التنبؤ بالخصائص الطوبولوجية لمتغصنات النانوستار، مثل الوزن الجزيئي والحجم. في هذه المقالة ، قمنا بحساب مؤشر زغرب الأول ، ومؤشر زغرب الثاني ، ومؤشر زغرب الثالث ، ومؤشر سومبور ، ومؤشر اتصال رابطة الذرة ، ومؤشر نيرمالا ، ومؤشر التوافقي لعائلتين جديدتين من التشعبات النانوية مثل NS_1 والمعروف بأسم مونومر دي استر الامينو ايزوفيثالات و PD_1 والمعروف بولي اميدو امين .