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On Sombor Index and Domination Number of Graphs

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Abstract

Recently I. Gutman [4] put forward a novel topological index namely the Sombor index. Motivated by this novel index, we study the new variants of Sombor index and to examine the correlation of newly introduced topological indices we have computed the values of these indices by taking all possible trees on 10 vertices. Further, we compute bounds for certain nanostructures viz. hexagonal parallelogram $P(m,n)$-nanotube, triangular benzenoid G_n, zigzag-edge coronoid fused with starphene nanotubes $ZCS(k,l,m)$, dominating derived networks D_1, D_2, D_3, Porphyrin Dendrimer, Zinc-Porphyrin Dendrimer, Propyl Ether Imine Dendrimer, Poly(Ethylene amido amine Dendrimer, PAMAM dendrimers(PD_1, PD_2, DS_1), linear polyomino chain $L_n, Z_n, B_n^1 (n \geq 3)$ $B_n^2 (n \geq 4)$ and triangular, hourglass, and jagged-rectangle benzenoid systems in terms of Sombor index and domination number.

Keywords: Sombor index; trees; nanostructures; dendrimers.
Subject Classification: 05C90; 05C35; 05C12.

1 Introduction

All graphs considered in this paper are finite, simple and undirected. In particular, these graphs do not possess loops. Let $G = (V, E)$ be a graph with the vertex set $V(G) = \{v_1, v_2, v_3, \dots \dots .. v_n\}$ and the edge set $E(G) = \{e_1, e_3, \dots \dots .. e_m\}$, that is $|V(G)| = n$ and $|E(G)| = m$. The vertex u and v are adjacent if $uv \in E(G)$. The open(closed) neighborhood of a vertex $v \in V(G)$ is $N(v) = \{u : uv \in E(G)\}$ and $N[v] = N(v) \cup \{v\}$ respectively. The degree of a vertex $v \in V(G)$ is denoted by $d_G(v)$ and is defined as $d_G(v) = |N(v)|$. A vertex $v \in V(G)$ is pendant if $|N(v)| = 1$ and is called support vertex if it is adjacent to pendant vertex. Any vertex $v \in V(G)$ with $|N(v)| > 1$ is called internal vertex. If $d_G(v) = r$ for every vertex $v \in V(G)$, where $r \in \mathbb{Z}^+$ then G is called r-regular. If $r = 2$ then it is called cycle graph C_n and for $r = 3$ it is called the cubic graph. A graph G

is unicyclic If $|V| = |E|$. For undefined terminologies we refer the reader to [7].

Molecular descriptors give hope that the journey throughout endless chemical space won't be a random wandering but a methodical voyage toward substances of importance to mankind. Nowadays, there is a myriad of molecular descriptors, and among them, the topological indices have a prominent place. Topological index is simply a numeric associated with the molecular graph. So far, large number of such quantities are put forward by many researchers right from 1972 [3]. An useful topological index is one which has a good predicting power in QSPR studies. Therefore, topological indices can be categorized into two categories useful and not so useful TI's. One of the most useful topological index is the Sombor index $SO(G)$ which is put forward by I Gutman[4]:

$$SO(G) = \sum_{uv\in E(G)} [\sqrt{deg(u)^2 + deg(v)^2}] \quad (1)$$

Motivated by the Sombor index, here we put forward the variants of Sombor index as follows:

$$SO'(G) = \sum_{uv\in E(G)} [deg(u)^2 \times deg(v)^2] \quad (2)$$

$$N_{SO}(G) = \sum_{uv\in E(G)} [\sqrt{deg(S_u)^2 + deg(S_v)^2}] \quad (3)$$

$$N'_{SO}(G) = \sum_{uv\in E(G)} [deg(S_u)^2 \times deg(S_v)^2] \quad (4)$$

where $deg(S_u)(G)$ is the sum of the degrees of neighborhood vertices of u in G. For more detail on topological indices refer [5-6,11-12,14-15].

2 Quality of Sombor Index and its Variants

Many papers are dealing with the "quality of topological descriptors". This is a vague term, which is viewed and defined differently by many researchers. There were attempts to unify these approaches and to gather a set of requirements that a novel topological invariant should fulfill. One of the best known in the circles of chemical graph theorists, and commonly quoted, is the Randic'[13] set of qualities that a novel topological descriptor should possess. There, Randic compiled a list of thirteen tests to which a novel topological index should be subjected. If it would successfully pass these tests, then it would be qualified for further and deeper investigations. Some of these tests are of pure chemical nature, while some of them are technical, which almost all topological indices fulfill.

2.1 Correlations of Sombor Index with its Variants

Reasons for introducing novel topological indices, which are highly correlated with other similar indices, are quite difficult to understand because almost all structural features of the underlying graph can be harvested with the already existing invariants. Therefore, it is of utmost importance to check whether the correlations of a novel descriptor with other similar indices are exceeding the permitted upper limits. The above mentioned topological indices were calculated for all trees with 10 vertices(see [7]), calculated sombor index and its invariants and obtained correlations are given in the below.

Table 1. Sombor index and its variants values for all trees with 10 vertices.

Tree	$SO(T)$	$SO'(T)$	$N_{SO}(T)$	$N'_{SO}(T)$
T_1	24.2711	32	45.495	116
T_2	26.3083	34	43.3822	130
T_3	25.7159	32	48.6852	129
T_4	26.1592	35	47.4309	122
T_5	26.0101	36	50.4726	140
T_6	26.1592	35	49.9902	141
T_7	26.0101	36	46.7485	151
T_8	26.0101	36	45.8926	140
T_9	30.3912	38	54.1498	164
T_{10}	30.1479	34	57.5761	182
T_{11}	29.7988	36	57.5229	189
T_{12}	29.9045	42	61.0732	202
T_{13}	29.9045	42	60.5761	208
T_{14}	28.0175	42	64.7709	222
T_{15}	36.5025	44	60.3884	200
T_{16}	36.1963	47	67.917	254
T_{17}	36.1963	47	68.0484	257
T_{18}	35.8901	50	73.3683	283
T_{19}	30.9559	44	78.8602	309
T_{20}	44.6312	52	97.0892	316
T_{21}	44.2807	56	81.3734	356
T_{22}	43.6883	54	79.6742	368
T_{23}	54.7710	62	88.9148	441
T_{24}	54.3876	67	97.5843	491
T_{25}	50.7935	58	106.2385	603
T_{26}	81.4984	81	114.55	729
T_{27}	26.4930	36	51.2693	144
T_{28}	25.4177	37	52.9866	152
T_{29}	28.1834	38	54.6509	163
T_{30}	28.0473	38	47.5545	136
T_{31}	28.6396	33	52.8837	155
T_{32}	28.1964	37	52.9320	156
T_{33}	28.0473	38	54.626	167
T_{34}	24.4417	38	54.6652	164
T_{35}	25.2188	32	56.3682	173
T_{36}	28.0473	38	54.6561	162
T_{37}	28.1964	37	56.4096	174
T_{38}	27.9072	39	56.4038	172
T_{39}	27.9072	39	56.3418	165
T_{40}	27.9072	39	56.3951	174

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T_{41}	27.8982	39	58.1842	184
T_{42}	27.7582	40	56.9302	174
T_{43}	27.6091	41	58.7240	184
T_{44}	32.4284	40	57.0369	178

Tree	$SO(T)$	$SO'(T)$	$N_{SO}(T)$	$N'_{SO}(T)$
T_{45}	32.2793	37	60.0142	188
T_{46}	32.1850	42	60.3162	198
T_{47}	32.2793	41	58.7525	191
T_{48}	32.1850	42	60.5030	202
T_{49}	32.1302	42	60.3977	201
T_{50}	32.0359	43	62.2377	208
T_{51}	31.9417	44	63.9989	219
T_{52}	23.0972	40	63.0661	222
T_{53}	31.9358	44	63.7966	218
T_{54}	31.8809	44	63.9201	221
T_{55}	31.7867	45	65.6661	227
T_{56}	31.6924	46	67.4935	238
T_{57}	31.6376	46	67.5749	209
T_{58}	31.7867	45	65.8153	228
T_{59}	31.5434	47	69.3628	205
T_{60}	31.4491	44	103.586	255
T_{61}	38.5397	46	65.4695	241
T_{62}	38.3906	47	67.3811	251
T_{63}	38.2335	49	67.7562	251
T_{64}	38.0593	46	72.4539	281
T_{65}	37.9022	52	76.0151	301
T_{66}	37.9102	51	62.7295	216
T_{67}	32.3679	53	76.9612	308
T_{68}	37.5960	55	81.5069	327
T_{69}	56.5985	54	77.3483	333
T_{70}	46.1259	59	85.8494	383
T_{71}	45.9244	62	91.0780	413
T_{72}	56.3667	69	100.112	513
T_{73}	36.5113	44	62.5245	216
T_{74}	36.2680	46	66.2609	236
T_{75}	35.5656	52	76.7989	293
T_{76}	35.5656	52	76.7290	252
T_{77}	35.8090	50	73.0192	276
T_{78}	42.6226	50	71.5626	279

T_{79}	41.5954	58	85.1560	271
T_{80}	43.4196	59	86.9025	333
T_{81}	49.9942	66	96.3577	459
T_{82}	47.8632	65	91.1115	441
T_{83}	29.8044	42	61.0622	201
T_{84}	29.2120	40	61.5342	200
T_{85}	31.2186	42	61.0545	197
T_{86}	29.6553	43	62.7823	207
T_{87}	29.6553	43	63.1326	205
T_{88}	29.9444	41	59.2292	191
T_{89}	29.9444	41	59.1821	187
T_{90}	29.9444	41	59.2813	188
T_{91}	30.0935	40	57.4647	177
T_{92}	30.2335	39	45.8736	177
T_{93}	32.9525	52	73.9957	271
T_{94}	33.5746	49	72.0852	237
T_{95}	33.9730	46	66.7222	235
T_{96}	28.1170	47	68.6798	245
T_{97}	33.6838	48	70.3820	239
T_{98}	33.7781	47	68.5687	242
T_{99}	34.1764	44	63.2115	215
T_{100}	34.0672	45	64.8992	225
T_{101}	43.4815	61	84.1534	345
T_{102}	37.9009	51	74.3867	279
T_{103}	37.5969	54	79.2030	309
T_{104}	31.7015	45	65.8726	225
T_{105}	31.7015	45	65.6594	221
T_{106}	39.9565	53	77.2554	305

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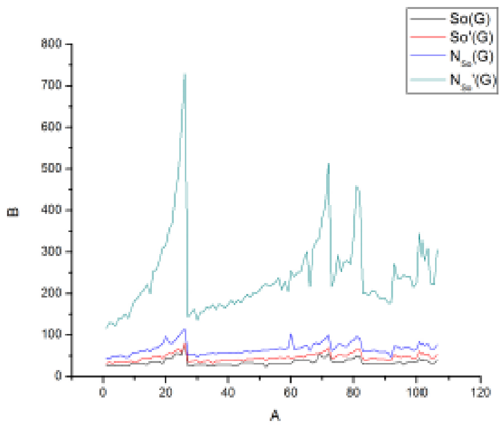
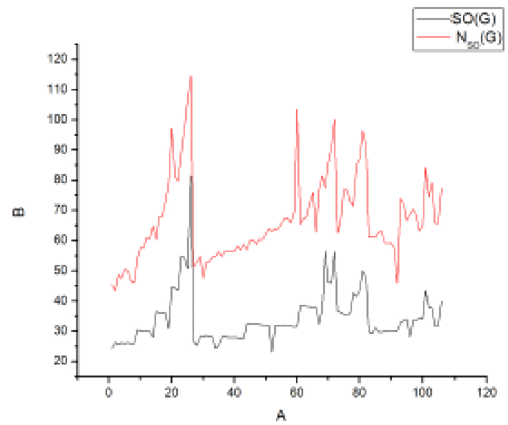
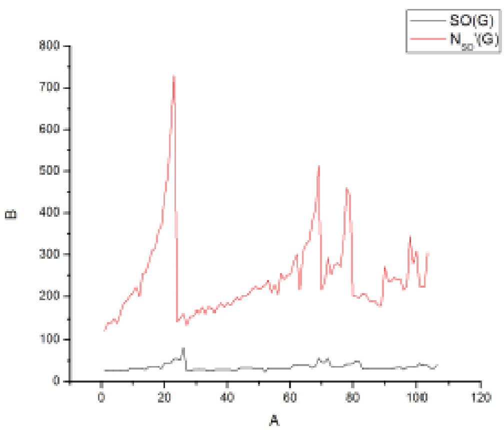
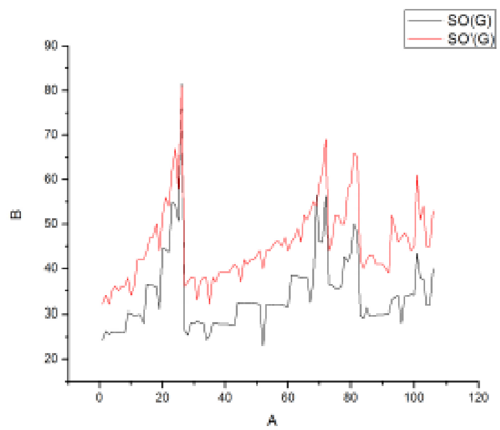
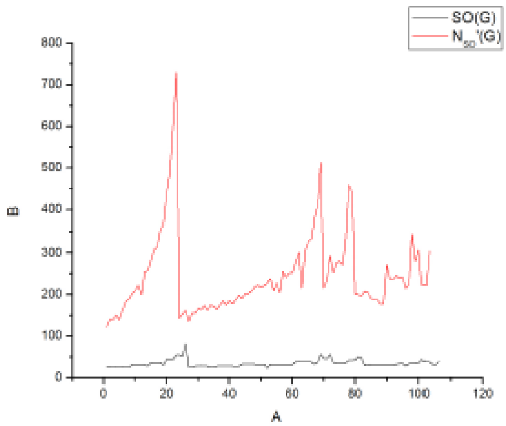
In the following figures, the correlation of Sombor index with its variants are depicted:

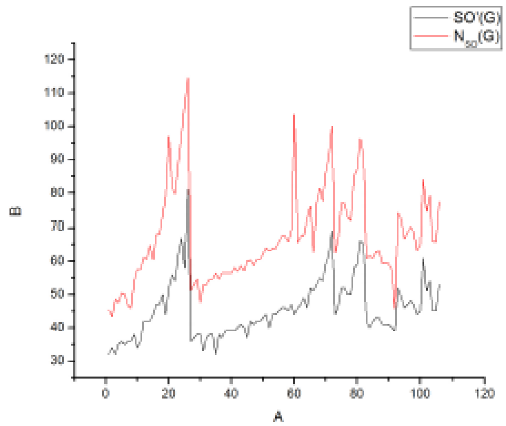


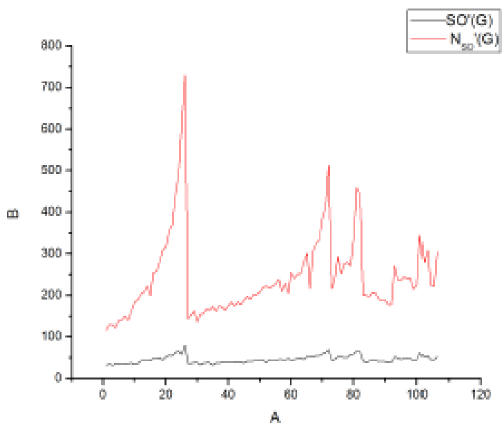


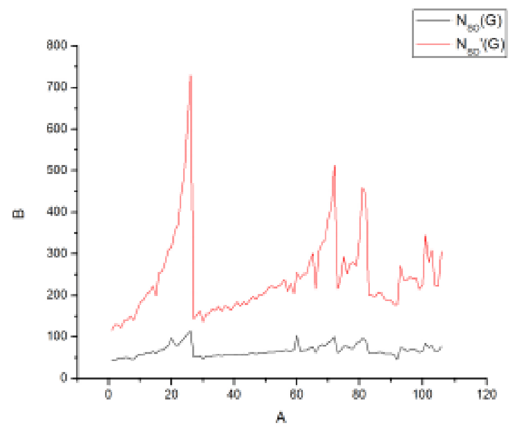












From above figures and Table 1, it is clear that the Sombor index is not correlated well with other variants. Therefore, it reflects that the other variants of Sombor index can be used for QSPR analysis to check their predicting power.

3 Nanostructures

In this section we consider the chemical structures like hexagonal parallelogram $P(m,n)$ -nanotube, triangular benzenoid G_n zigzag-edge coronoid fused with starphene nanotubes $ZCS(k,l,m$([2]), dominating derived networks D_1, D_2, D_3([1]), Porphyrin Dendrimer, Zinc-Porphyrin Dendrimer, Propyl Ether Imine Dendrimer, Poly(Ethylene amido amine Dendrimer, PAMAM dendrimers(PD_1, PD_2, DS_1)([8]), linear polyomino chain L_n, Z_n, $B_n^1(n \geq 3)$, $B_n^2(n \geq 4)$([9]) and triangular, hourglass, and jagged-rectangle benzenoid systems([10]).

In this paper, we consider the chemical structures like hexagonal parallelogram $P(m,n)$ -nanotube, triangular benzenoid G_n , zigzag-edge coronoid fused with starphene nanotubes $ZCS(k,l,m)$, dominating derived networks D_1, D_2, D_3 , Porphyrin Dendrimer,

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Zinc-Porphyrin Dendrimer, Propyl Ether Imine Dendrimer, Poly(Ethylene amido amine Dendrimer, PAMAM dendrimers(PD_1, PD_2, DS_1), linear polyomino chain L_n, Z_n, $B_n^1(n \geq 3)$, $B_n^2(n \geq 4)$ and triangular, hourglass, and jagged-rectangle benzenoid systems which are depicted in the following figures:

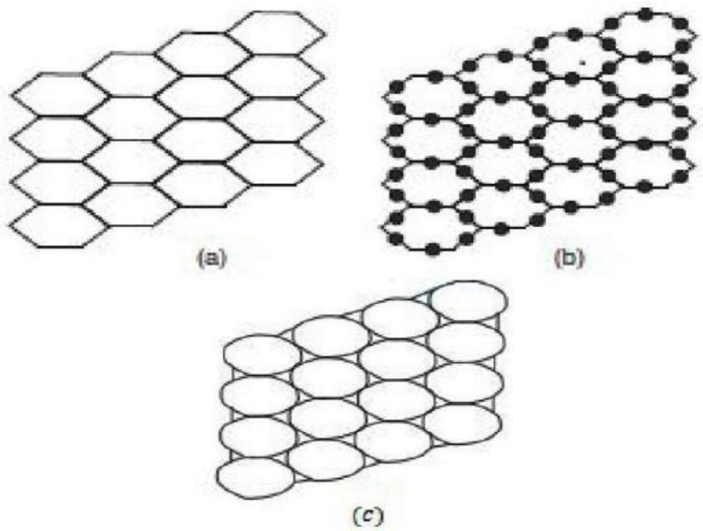

Figure 1: (a) A hexagonal parallelogram $P(4,4)$ (b) A subdivision of hexagonal parallelogram $P(4,4)$ (c) A line graph of subdivision graph of hexagonal parallelogram $P(4,4)$

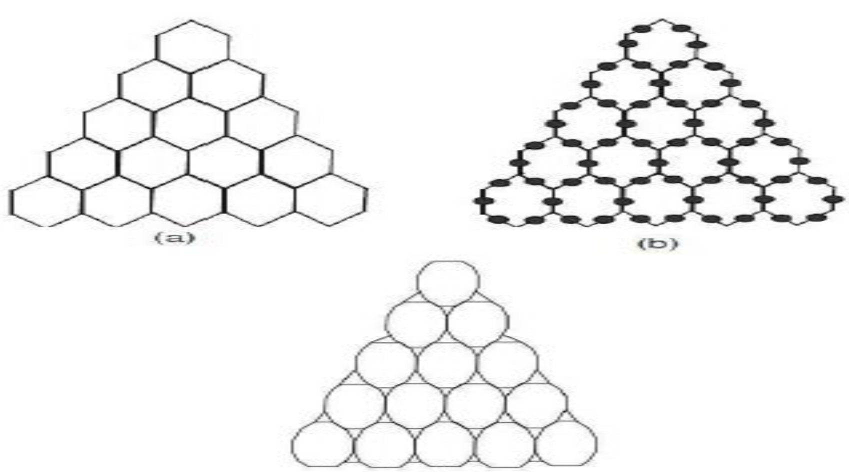

Figure 2: (a) Triangular Benzenoid G_n for $n = 5$(b) A subdivision of triangular Benzenoid G_n for $n = 5$ (c) Line graph of subdivision graph of triangular Benzenoid G_n for $n = 5$

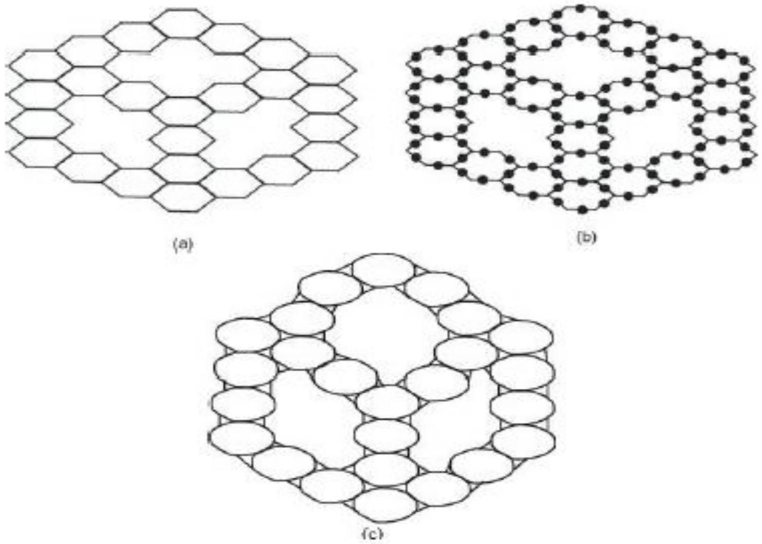

Figure 3: (a) The Zigzag-edge conronoid fused with starphene nanotubes $ZCS(k,l,m)$ for $k=l=m=4$ (b) The subdivision graph of zigzag-edge coronoid fused with starphene nanotubes $ZCS(k,l,m)$ for $k=l=m=4$ (c) The line graph of the subdivision graph of zigzag-edge coronoid fused with starphene nanotubes $ZCS(k,l,m)$ for $k=l=m=4$

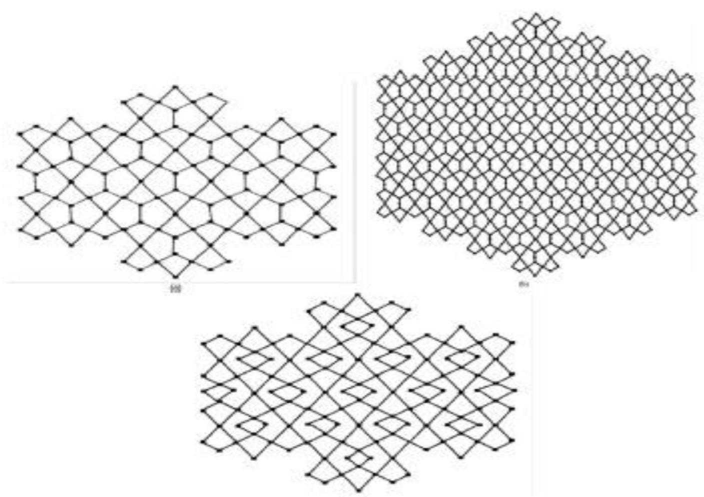

Figure 4: (a) Dominating derived network of first type $D_1(2)$ (b) Dominating derived network of second type $D_2(4)$ (c)Dominating derived network of third type $D_3(n)$

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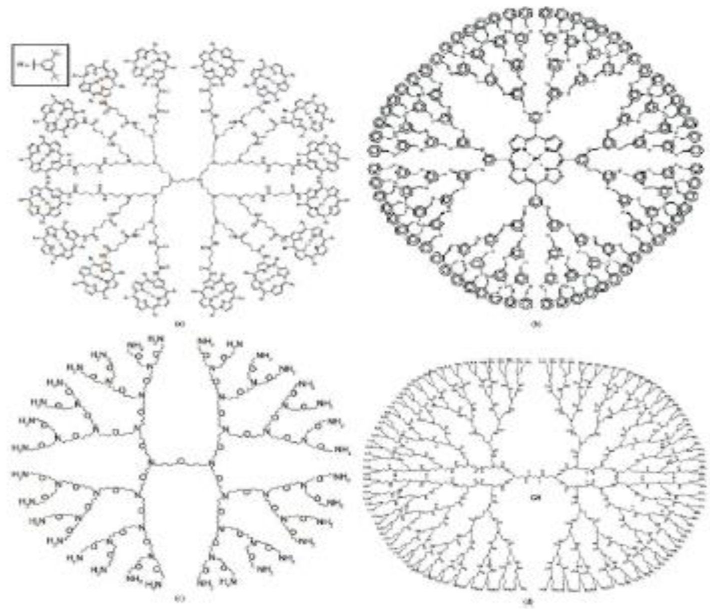

Figure 5: (a) Porphyrin dendrimer (b) Zinc-Porphyrin dendrimer (c) Propyl ether imine dendrimer (d) polyethelene amido amine dendrimer

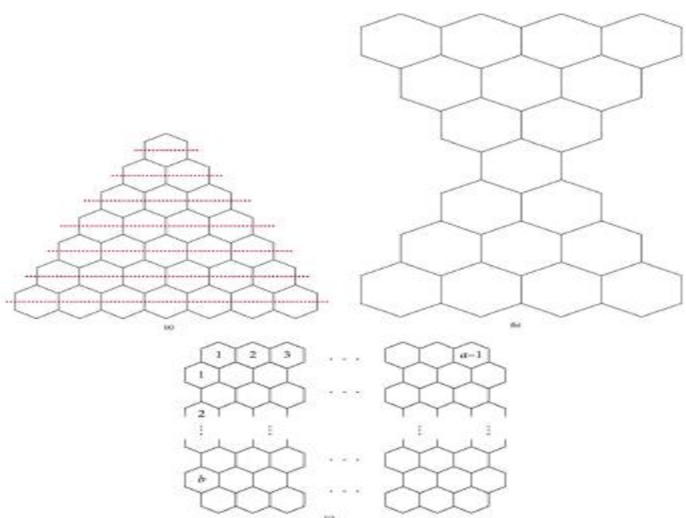

Figure 6: (a)Triangular benzoid (b) Benzoid hourglass system (c) Benzoid jagged-rectangle system

Theorem 1 *Let G denotes the line graph of subdivision graph of the hexagonal parallelogram, then*

$SO(G) \leq (m+n+mn) + 2\sqrt{8}(m+n+4) + 4\sqrt{13}(m+n-2) + \sqrt{18}(9mn-2m-2n-5)$

$SO'(G) \leq (3mn+2m+2n+1) + 8(m+n+4) + 24\sqrt{13}(m+n-2) + 9(9mn-2m-2n-5)$

Proof. Let $P(m,n); m,n \in \mathbb{Z}^+$ be a hexagonal parallelogram of order $2(m+n+mn)$ and size$(3mn+2m+2n+1)$ respectively. Let $G = L(S(P(m,n)))$ denote the line graph of subdivision graph of $P(m,n)$; $m,n \in \mathbb{Z}^+$ then clearly, the order and size of G are 2(3mn+2m+2n+1) and $(9mn+4m+4n+5)$ respectively.

Since, for any connected graph

$\gamma(G) \leq \frac{n}{2}$

.

Therefore, we have

$$\gamma(SO(G)) \leq \frac{2(m+n+mn)}{2} = m+n+mn \qquad (5)$$

Also,

$$\gamma(SO'(G)) \leq \frac{2(3mn+2m+2n+1)}{2} = 3mn+2m+2n+1. \qquad (6)$$

The edge set of G can be partitioned into three disjoint sets $\varepsilon_{2,2}$, $\varepsilon_{2,3}$ and $\varepsilon_{3,3}$, where $\varepsilon(L(S(P(m,n)))) = \varepsilon_{2,2} \cup \varepsilon_{2,3} \cup \varepsilon_{3,3}$. Further, $|\varepsilon_{2,2}I = 2(m+n+4)$, $|\varepsilon_{2,3}| = 4(m+n-2)$, $\varepsilon_{3,3}| = 9mn-2m-2n-5.$ Such that $|\varepsilon(L(S(P(m,n))))| = |\varepsilon_{2,2}| + |\varepsilon_{2,3}| + |\varepsilon_{3,3} = 9mn+4m+4n+5.$ Thus, employing equations (1)-(2) and (5)-(6) we get the required result.

Theorem 2 *Let $L(S(G_n))$ denotes the line graph of subdivision graph of the hexagonal parallelogram, then*

$SO(G) \leq \frac{n^2+4n+1}{2} + 3\sqrt{8}(n+3) + 6\sqrt{13}(n-1) + 3\sqrt{18}\frac{3n^2+n-4}{2}$

$SO'(G) \leq \frac{3n(n+3))}{2} + 12(n+3) + 36(n-1) + 27\frac{3n^2+n-4}{2}$

Proof. Let $G_n; n \in \mathbb{Z}^+$ be a triangular benzenoid of order n^2+4n+1 and size $\frac{3}{2}n(n+3)$ respectively. Let $L(S(G_n)))$ denote the line graph of subdivision graph of G_n then clearly, the order and size of $L(S(G_n)))$ are $3n(n+3)$ and $\frac{3(3n^2+7n+2)}{2}$ respectively.

Since, for any connected graph

$$\gamma(G) \le \frac{n}{2}$$

.

Therefore, we have

$$\gamma(SO(G)) \le \frac{n^2+4n+1}{2}. \quad (7)$$

Also,

$$\gamma(SO'(G)) \le \frac{3n(n+3))}{2}. \quad (8)$$

The edge set of $L(S(G_n)))$ can be partitioned into three disjoint sets $\varepsilon_{2,2}, \varepsilon_{2,3}$ and $\varepsilon_{3,3}$, where $\varepsilon(L(S(G_n)))) = \varepsilon_{2,2} \cup \varepsilon_{2,3} \cup \varepsilon_{3,3}$. Further, $|\varepsilon_{2,2} = 3(n+3)$, $|\varepsilon_{2,3}| = 6(n-1)$, $|\varepsilon_{3,3}| = \frac{3(3n^2+n-4)}{2}$. Such that $|\varepsilon(L(S(G_n)))| = |\varepsilon_{2,2}| + |\varepsilon_{2,3}| + |\varepsilon_{3,3}| = \frac{3(3n^2+7n+2)}{2}$. Thus, employing equations (1)-(2) and (7)-(8) we get the required result.

Theorem 3 *Let $L(S(I))$ be the line graph of the subdivision graph of zigzag-edge coronoid fused with starphene nanotubes $ZCS(k,l,m)$ for $k = l = m = 4$. Then*

$$SO(G) \le (18k+26) + 6\sqrt{8}(k+l+m-5) + 12\sqrt{13}(k+l+m-7) + 21\sqrt{18}((k+l+m)-39)$$

$$SO'(G) \le 15(k+l+m+126) + 24(k+l+m-5) + 72(k+l+m-7) + 189\sqrt{18}((k+l+m)-39)$$

Proof. Let I be zigzag-edge coronoid fused with starphene nanotubes $ZCS(k,l,m)$ for $k = l = m = 4$ of order $36k + 54$ and size $15(k+l+m) - 63$ respectively. Let $L(S(I))$ be the line graph of the subdivision graph of zigzag-edge coronoid fused with starphene nanotubes $ZCS(k,l,m)$ for $k = l = m = 4$. Then clearly, the order and size of $L(S(I))$ are $30(k+l+m\ \ )126)$ and $39(k+l+m) + 153$. respectively. Since, for any connected graph

$$\gamma(G) \le \frac{n}{2}$$

.

Therefore, we have

$$\gamma(SO(G)) \le \frac{36k+54}{2} = (18k+26). \quad (9)$$

Also,

$$\gamma(SO'(G)) \le \frac{30(k+l+m126)}{2} = 15(k+l+m+126). \quad (10)$$

The edge set of $L(S(I))$ can be partitioned into three disjoint sets $\varepsilon_{2,2}$, $\varepsilon_{2,3}$ and $\varepsilon_{3,3}$, where $\varepsilon(L(S(I))) = \varepsilon_{2,2} \cup \varepsilon_{2,3} \cup \varepsilon_{3,3}$. Further, $|\varepsilon_{2,2}| = 6(k+l+m-5)$, $|\varepsilon_{2,3}| = 12(k+l+m-7)$, $|\varepsilon_{3,3}| = 21(k+l+m) - 39$. Such that $|\varepsilon(L(S(I)))| = |\varepsilon_{2,2}| + |\varepsilon_{2,3}| + |\varepsilon_{3,3}| = 39(k+l+m) + 153$. Thus, employing equations (1)-(2) and (9)-(10) we get the required result.

Theorem 4 *Let $D_1(n)$ be the dominating derived network of 1st type. Then*

$$SO(D_1(n)) \leq \frac{O(D_1(n))}{2} + 4\sqrt{8}n + \sqrt{13}(4n-4) + \sqrt{20}(28n-16) + \sqrt{18}(9n^2-13n+5)$$
$$+5(36n^2-56m+24) + \sqrt{32}(36n^2-52n+20)$$
$$SO'(D_1(n)) \leq \frac{O(D_1(n))}{2} + \frac{49}{100}n^2 + \frac{19}{25}n - \frac{8}{25}.$$

Proof. Let $D_1(n)$ be the dominating derived network of 1st type. Since, for any connected graph

$$\gamma(G) \leq \frac{n}{2}$$

.

Therefore, we have

$$\gamma(SO(D_1(n))) \leq \frac{O(D_1(n))}{2}. \quad (11)$$

Also,

$$\gamma(SO'(D_1(n))) \leq \frac{O(D_1(n))}{2}. \quad (12)$$

The edge set of $D_1(n)$ can be partitioned into six disjoint sets $\varepsilon_{2,2}, \varepsilon_{2,3}, \varepsilon_{2,4}, \varepsilon_{3,3}, \varepsilon_{3,4}$ and $\varepsilon_{4,4}$, where $\varepsilon(D_1(n)) = \varepsilon_{2,2} \cup \varepsilon_{2,3} \cup \varepsilon_{2,4} \cup \varepsilon_{3,3} \cup \varepsilon_{3,4} \cup \varepsilon_{4,4}$. Further, $|\varepsilon_{2,2}| = 4n$, $|\varepsilon_{2,3}| = 4n-4$, $|\varepsilon_{2,4}| = 28n-16$, $|\varepsilon_{3,3}| = [\ 9n^2-13n+5$, $|\varepsilon_{3,4}| = 36n^2-56n+24$ and $|\varepsilon_{4,4}| = 36n^2-52n+20$. Such that $|\varepsilon(D_1(n))| = |\varepsilon_{2,2}| + |\varepsilon_{2,3}| + |\varepsilon_{2,4}|[\ + |\varepsilon_{3,3}| + |\varepsilon_{3,4}| + |\varepsilon_{4,4}|$. Thus, employing equations (1)-(2) and (11)-12 we get the required result.

Theorem 5 *Let $D_2(n)$ be the dominating derived network of 2nd type. Then*

$$SO(D_2(n)) \leq \frac{O(D_2(n))}{2} + 4\sqrt{8}n + \sqrt{13}(18n^2-22n+6) + \sqrt{20}(28n-16) + 5(36n^2-56n+24)$$
$$+\sqrt{32}(36n^2-52n+20)$$
$$SO'(D_2(n)) \leq \frac{O(D_2(n))}{2} + 16n + 6(18n^2-22n+6) + 8(28n-16) + 12(36n^2-56n+24)$$
$$+16(36n^2-52n+20)$$

Proof. Let $D_2(n)$ be the dominating derived network of 2nd type. Since, for any connected graph

$\gamma(G) \leq \frac{n}{2}$

.

Therefore, we have

$$\gamma(SO(D_2(n))) \leq \frac{O(D_2(n))}{2}. \quad (13)$$

Also,

$$\gamma(SO'(D_2(n))) \leq \frac{O(D_2(n))}{2}. \quad (14)$$

The edge set of $D_2(n)$ can be partitioned into five disjoint sets $\varepsilon_{2,2}, \varepsilon_{2,3}, \varepsilon_{2,4}, \varepsilon_{3,4}$ and $\varepsilon_{4,4}$, where $\varepsilon(D_2(n)) = \varepsilon_{2,2} \cup \varepsilon_{2,3} \cup \varepsilon_{2,4} \cup \varepsilon_{3,4} \cup \varepsilon_{4,4}$. Further, $|\varepsilon_{2,2}| = 4n$, $|\varepsilon_{2,3}| = 18n^2 - 22n + 6$, $|\varepsilon_{2,4}| = 28n - 16$, $|\varepsilon_{3,4} = 36n^2 - 56n + 24$ and $|\varepsilon_{4,4}| = 36n^2 - 52n + 20$. Such that $|\varepsilon(D_2(n))| = |\varepsilon_{2,2}| + |\varepsilon_{2,3}| + \varepsilon_{2,4}| + |\varepsilon_{3,4}| + |\varepsilon_{4,4}|$. Thus, employing equations (1)-(2) and (13)-(14) we get the required result.

Theorem 6 *Let $D_3(n)$ be the dominating derived network of 3rd type. Then*

$$SO(D_3(n)) \leq \frac{O(D_3(n))}{2} + 4\sqrt{8}n + \sqrt{20}(36n^2 - 20n) + \sqrt{32}(72n^2 - 108n + 44)$$

$$SO'(D_3(n)) \leq \frac{O(D_3(n))}{2} + 16n + 8(36n^2 - 20n) + 16(72n^2 - 108n + 44)$$

Proof. Let $D_3(n)$ be the dominating derived network of 3rd type. Since, for any connected graph

$\gamma(G) \leq \frac{n}{2}$

.

Therefore, we have

$$\gamma(SO(D_3(n))) \leq \frac{O(D_3(n))}{2}. \quad (15)$$

Also,

$$\gamma(SO'(D_3(n))) \leq \frac{O(D_3(n))}{2}. \quad (16)$$

The edge set of $D_1(n)$ can be partitioned into three disjoint sets $\varepsilon_{2,2}$ $\varepsilon_{2,4}$ and $\varepsilon_{4,4}$, where $\varepsilon(D_3(n)) = \varepsilon_{2,2} \cup \varepsilon_{2,4} \cup \varepsilon_{4,4}$. Further, $|\varepsilon_{2,2}| = 4n$, $|\varepsilon_{2,4}| = 36n^2 - 20n$ and $|\varepsilon_{4,4} = 72n^2 - 108n + 44$. Such that $|\varepsilon(D_3(n))| = |\varepsilon_{2,2}| + |\varepsilon_{2,4}| + |\varepsilon_{4,4}|$. Thus, employing equations (1)-(2) and (15)-(16) we get the required result.

Theorem 7 *Let D_nP_n be the prophyrin dendrimer. Then*

$$SO(D_nP_n) \leq (48n - 5) + 2\sqrt{10}n + 24\sqrt{17}n + \sqrt{8}(10n - 5) + \sqrt{13}(48n - 6) + 13\sqrt{18}n + 40n$$

$$SO'(D_nP_n) \leq (48n - 5) + 315n + 4(10n - 5) + 6(48n - 6)$$

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Proof. Let D_nP_n be the prophyrin dendrimer of order $96n-10$ and size $105n-11$ respectively. Since, for any connected graph

$$\gamma(G) \leq \frac{n}{2}$$

.

Therefore, we have

$$\gamma(SO(D_nP_n) \leq \frac{96n-10}{2} = (48n-5). \quad (17)$$

Also,

$$\gamma(SO'(D_nP_n) \leq \frac{O(D_3(n))}{2} = (48n-5). \quad (18)$$

The edge set of D_nP_n can be partitioned into six disjoint sets $\varepsilon_{1,3}$, $\varepsilon_{1,4}$, $\varepsilon_{2,2}$, $\varepsilon_{2,3}$, $\varepsilon_{3,3}$ and $\varepsilon_{3,4}$, where $\varepsilon(D_nP_n) = \varepsilon_{1,3} \cup \varepsilon_{1,4} \cup \varepsilon_{2,2} \cup \varepsilon_{2,3} \cup \varepsilon_{3,3} \cup \varepsilon_{3,4}$. Further, $|\varepsilon_{1,3}| = 2n$, $|\varepsilon_{1,4}| = 24n$, $|\varepsilon_{2,2}| = 10n-5$, $|\varepsilon_{2,3}| = 48n-6$, $|\varepsilon_{3,3}| = 13n$ and $|\varepsilon_{3,4}| = 8n$. Such that $|\varepsilon(D_nP_n)| = |\varepsilon_{1,3}| + |\varepsilon_{1,4}| + |\varepsilon_{2,2}| + |\varepsilon_{2,3}| + |\varepsilon_{3,3} + |\varepsilon_{3,4}| = 105n-11$. Thus, employing equations (1)-(2) and (17)-(18) we get the required result.

Theorem 8 *Let DPZ_n be the Zinc-Porphyrin dendrimer. Then*

$$SO(DPZ_n) \leq (48n-5) + 16\sqrt{8}\cdot 2^n + \sqrt{13}(40\cdot 2^n - 16) + \sqrt{18}(8\cdot 2^n - 16) + 20$$

$$SO'(DPZ_n) \leq (48n-5) + 64\cdot 2^n + 6(40\cdot 2^n - 16) + 9(8\cdot 2^n - 16) + 48$$

Proof. Let DPZ_n be the Zinc-Porphyrin dendrimer. of order $96n-10$ and size $105n-11$ respectively. Since, for any connected graph

$$\gamma(G) \leq \frac{n}{2}$$

.

Therefore, we have

$$\gamma(SO(DPZ_n) \leq \frac{96n-10}{2} = (48n-5). \quad (19)$$

Also,

$$\gamma(SO'(DPZ_n) \leq \frac{O(D_3(n))}{2} = (48n-5). \quad (20)$$

The edge set of DPZ_n can be partitioned into four disjoint sets $\varepsilon_{2,2}$, $\varepsilon_{2,3}$, $\varepsilon_{3,3}$ and $\varepsilon_{3,4}$, where $\varepsilon(DPZ_n) = \varepsilon_{2,2} \cup \varepsilon_{2,3} \cup \varepsilon_{3,3} \cup \varepsilon_{3,4}$. Further, $|\varepsilon_{2,2}| = 16\cdot 2^n - 4$, $|\varepsilon_{2,3}| = 40\cdot 2^n - 16$, $|\varepsilon_{3,3} = 8\cdot 2^n - 16$ and $|\varepsilon_{3,4}| = 4$. Such that $|\varepsilon(DPZ_n)| = |\varepsilon_{2,2}|[+ |\varepsilon_{2,3}| + |\varepsilon_{3,3}|[+[|\varepsilon_{3,4}| = 105n-11$. Thus, with this background by employing equations (1)-(2) and (19)-(20), we get the required results.

Theorem 9 *For the PAMAM dendrimers PD_1, we have*

$$SO(PD_1) \leq \frac{O(PD_1)}{2} + 3\sqrt{5}\cdot 2^n + \sqrt{10}(6\cdot 2^n - 3) + \sqrt{8}(18\cdot 2^n - 9) + \sqrt{13}(21\cdot 2^n - 12)$$

$SO'(PD_1) \leq \frac{O(PD_1)}{2} + 6 \cdot 2^n + 3(6 \cdot 2^n - 3) + 4(18 \cdot 2^n - 9) + 6(21 \cdot 2^n - 12)$

Proof. Let PD_1 denote PAMAM dendrimers with tri-functional core unit generated by G_n with n growth stages. Since, for any connected graph

$$\gamma(G) \leq \frac{n}{2}$$

.

Therefore, we have

$$\gamma(SO(PD_1)) \leq \frac{O(PD_1)}{2}. \quad (21)$$

Also,

$$\gamma(SO'(PD_1) \leq \frac{O(PD_1)}{2}. \quad (22)$$

The edge set of PD_1 can be partitioned into four disjoint sets $\varepsilon_{1,2}$, $\varepsilon_{1,3}$, $\varepsilon_{2,2}$ and $\varepsilon_{2,3}$, where $\varepsilon(PD_1) = \varepsilon_{1,2} \cup \varepsilon_{1,3} \cup \varepsilon_{2,2} \cup \varepsilon_{2,3}$. Further, $|\varepsilon_{1,2}| = 3 \cdot 2^n$, $|\varepsilon_{1,3}| = 6 \cdot 2^n - 3$, $|\varepsilon_{2,2}| = 18.2^n - 9$ and $|\varepsilon_{2,3}| = 21 \cdot 2^n - 12$. Such that $|\varepsilon(PD_1)| = |\varepsilon_{1,2}| + |\varepsilon_{1,3}| + |\varepsilon_{2,2}| + |\varepsilon_{2,3}$. Thus, with this background by employing equations (1)-(1) and (21)-(22), we get the required results.

Theorem 10 *For the PAMAM dendrimers PD_2, we have*

$SO(PD_2) \leq \frac{O(PD_2)}{2} + 4\sqrt{5} \cdot 2^n + \sqrt{10}(8 \cdot 2^n - 4) + \sqrt{8}(24 \cdot 2^n - 11) + \sqrt{13}(28 \cdot 2^n - 14)$

$SO'(PD_2) \leq \frac{O(PD_2)}{2} + 8 \cdot 2^n + 3(8 \cdot 2^n - 4) + 4(24 \cdot 2^n - 11) + 6(28 \cdot 2^n - 14)$

Proof. Let PD_2 denote PAMAM dendrimers with different core unit generated by dendrimer G_n with n growth stages. Since, for any connected graph

$$\gamma(G) \leq \frac{n}{2}$$

.

Therefore, we have

$$\gamma(SO(PD_2)) \leq \frac{O(PD_2)}{2}. \quad (23)$$

Also,

$$\gamma(SO'(PD_2) \leq \frac{O(PD_2)}{2}. \quad (24)$$

The edge set of PD_2 can be partitioned into four disjoint sets $\varepsilon_{1,2}$, $\varepsilon_{1,3}, \varepsilon_{2,2}$ and $\varepsilon_{2,3}$, where $\varepsilon(PD_2) = \varepsilon_{1,2} \cup \varepsilon_{1,3} \cup \varepsilon_{2,2} \cup \varepsilon_{2,3}$. Further, $|\varepsilon_{1,2}| = 4 \cdot 2^n$, $|\varepsilon_{1,3}| = 8 \cdot 2^n - 4$, $|\varepsilon_{2,2}| = 24 \cdot 2^n - 11$ and $|\varepsilon_{2,3}| = 28.2^n - 14$. Such that $|\varepsilon(PD_2)| = |\varepsilon_{1,2}| + |\varepsilon_{2,2}| + |\varepsilon_{2,3}$. Thus, with this background by employing equations (1)-(2) and (23)-(24), we get the required results.

Theorem 11 *For the PAMAM dendrimers DS_1, we have*

$$SO(DS_1) \leq \frac{O(DS_1)}{2} + 4\sqrt{17} \cdot 3^n + \sqrt{8}(10 \cdot 3^n - 10) + \sqrt{20}(4 \cdot 3^n - 4)$$
$$SO'(DS_1) \leq \frac{O(DS_1)}{2} + 16\sqrt{17} \cdot 3^n + 4(10 \cdot 3^n - 10) + 8(4 \cdot 3^n - 4)$$

Proof. Let DS_1 denote PAMAM dendrimers with different core unit generated by dendrimer G_n with n growth stages. Since, for any connected graph
$$\gamma(G) \leq \frac{n}{2}$$
.

Therefore, we have

$$\gamma(SO(DS_1)) \leq \frac{O(DS_1)}{2}. \tag{25}$$

Also,
$$\gamma(SO'(DS_1) \leq \frac{O(DS_1)}{2}. \tag{26}$$

The edge set of DS_1 can be partitioned into three disjoint sets $\varepsilon_{1,4}, \varepsilon_{2,2}$ and $\varepsilon_{2,4}$, where $\varepsilon(DS_1) = \varepsilon_{1,4} \cup \varepsilon_{2,2} \cup \varepsilon_{2,4}$. Further, $|\varepsilon_{1,4}| = 4.3^n$, $|\varepsilon_{2,2}| = 10 \cdot 3^n - 10$, and $|\varepsilon_{2,4}| = 4 \cdot 3^n - 4$. Such that $|\varepsilon(DS_1) = |\varepsilon_{1,4}| + |\varepsilon_{2,2}| + \varepsilon_{2,4}|$. Thus, employing equations (1)-(2) and (25)-(26) we get the required result.

Theorem 12 *For a linear polyomino chain L_n we have*

$$SO(L_n) \leq \frac{O(L_n)}{2} + 2\sqrt{8} + 4\sqrt{13} + \sqrt{18}(3n - 5)$$
$$SO'(L_n) \leq \frac{O(L_n)}{2} + 9(3n - 5) + 32$$

Proof. Let L_n be the polyomino chain with n squares where $l_1 = n$ and $m = 1$. Since, for any connected graph
$$\gamma(G) \leq \frac{n}{2}$$
.

Therefore, we have

$$\gamma(SO(L_n)) \leq \frac{O(L_n)}{2}. \tag{27}$$

Also,
$$\gamma(SO'(L_n) \leq \frac{O(L_n)}{2}. \tag{28}$$

The edge set of L_n can be partitioned into three disjoint sets $\varepsilon_{2,2}$, $\varepsilon_{2,3}$ and $\varepsilon_{3,3}$, where $\varepsilon(L_n) = \varepsilon_{2,2} \cup \varepsilon_{2,3} \cup \varepsilon_{3,3}$. Further, $|\varepsilon_{2,2}| = 2$, $|\varepsilon_{2,3}| = 4$, and $|\varepsilon_{3,3}| = 3n - 5$. Such that $|\varepsilon(L_n)| = |\varepsilon_{2,2}| + |\varepsilon_{2,3}|[+|\varepsilon_{3,3}|$. Thus, employing equations (1)-(2) and

(27)-(28) we get the required results.

Theorem 13 *Let Z_n be zigzag polyomino chain with n squares such that $l_i = 2$ and $m = n-1$. Then*

$$SO(Z_n) \le \frac{O(Z_n)}{2} + 2\sqrt{20}(m-1) + \sqrt{32}(3n-2m-5) + 10 + 2\sqrt{8} + 4\sqrt{13}$$
$$SO'(Z_n) \le \frac{O(Z_n)}{2} + 16(m-1) + 16(3n-2m-5) + 32$$

Proof. Let Z_n be zigzag polyomino chain with n squares such that $l_i = 2$ and $m = n-1$. Polyomino chain consists of a sequence of segments $S_1, S_2, \ldots\ldots\ldots\ldots S_m$ and $l(S_i) = l_i$ where $m \ge 1$ and $i \in \{1,2, \cdots, m\}$. Since, for any connected graph

$$\gamma(G) \le \frac{n}{2}$$

.

Therefore, we have

$$\gamma(SO(Z_n)) \le \frac{O(Z_n)}{2}. \tag{29}$$

Also,

$$\gamma(SO'(Z_n) \le \frac{O(Z_n)}{2}. \tag{30}$$

The edge set of Z_n can be partitioned into five disjoint sets $\varepsilon_{2,2}, \varepsilon_{2,3}, \varepsilon_{2,4}, \varepsilon_{3,4}$ and $\varepsilon_{4,4}$, where $\varepsilon(Z_n) = \varepsilon_{2,2} \cup \varepsilon_{2,3} \cup \varepsilon_{2,4} \cup \varepsilon_{3,4} \cup \varepsilon_{4,4}$. Further, $|\varepsilon_{2,2}| = 2$, $|\varepsilon_{2,3}| = 4$, $|\varepsilon_{2,4}| = 2(m-1)$, $|\varepsilon_{3,4}| = 2$ and $|\varepsilon_{4,4}| = 3n-2m-5$. Such that $|\varepsilon(Z_n)| = |\varepsilon_{2,2}| + |\varepsilon_{2,3}| + |\varepsilon_{2,4}| + |\varepsilon_{3,4}| + |\varepsilon_{4,4}|$. Thus, employing equations (1)-(2) and (29)-(30) we get the required result.

Theorem 14 *For the polyomino chain with n squares and of m segments S_1 and S_2 satisfying $l_1 = 2$ and $l_2 = n-1$, $B_n^1(n \ge 3)$ we have the following:*

$$SO(B_n^1) \le \frac{O(B_n^1)}{2} + \sqrt{18}(3n-10) + 2\sqrt{8} + 5\sqrt{13} + \sqrt{20} + 15$$
$$SO'(B_n^1) \le \frac{O(B_n^1)}{2} + 9(3n-10) + 82$$

Proof. Let $B_n^1(n \ge 3)$ be the polyomino chain with n squares and m segments S_1 and S_2 satisfying $l_1 = 2$ and $l_2 = n-1$. Since, for any connected graph

$$\gamma(G) \le \frac{n}{2}$$

.

Therefore, we have

$$\gamma(SO(B_n^1)) \le \frac{O(B_n^1)}{2}. \tag{31}$$

Also,

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$$\gamma(SO'(B_n^1) \leq \frac{O(B_n^1)}{2}. \quad (32)$$

The edge set of $B_n^1(n \geq 3)$ can be partitioned into five disjoint sets $\varepsilon_{2,2}$, $\varepsilon_{2,3}$, $\varepsilon_{2,4}$, $\varepsilon_{3,3}$ and $\varepsilon_{3,4}$, where $\varepsilon(B_n^1(n \geq 3)) = \varepsilon_{2,2} \cup \varepsilon_{2,3} \cup \varepsilon_{2,4} \cup \varepsilon_{3,3} \cup \varepsilon_{3,4}$. Further, $|\varepsilon_{2,2}| = 2$, $|\varepsilon_{2,3}| = 5$, $|\varepsilon_{2,4}| =$ [1, $|\varepsilon_{3,3}| = 3n - 10$ and $|\varepsilon_{3,4}| = 3$. Such that $|\varepsilon(B_n^1(n \geq 3))| = |\varepsilon_{2,2}| + |\varepsilon_{2,3}| + |\varepsilon_{2,4}| + |\varepsilon_{3,3}| + |\varepsilon_{3,4}|$. Thus, with this background by employing equations (1)-(2) and (31)-(32), we get the required results.

Theorem 15 *For the polyomino chain with n squares and of m segments S_1, [$S_2, \cdots s_m$ satisfying $l_1 = l_m = 2$ and $l_2, l_3, \cdots, \geq 3$, $B_n^2(n \geq 4)$ we have the following:*

$$SO(B_n^2) \leq \frac{O(B_n^2)}{2} + \sqrt{18}(3n - 6m + 3) + 5(4m - 6) + 2\sqrt{13}m + 2\sqrt{8} + 2\sqrt{20}$$

$$SO'(B_n^2) \leq \frac{O(B_n^2)}{2} + 9(3n - 6m + 3) + 12(4m - 6) + 12m + 24$$

Proof. Let $B_n^2(n \geq 4)$ be the polyomino chain with n squares and m segments m segments $S_1, S_2, \cdots s_m$ satisfying $l_1 = l_m = 2$ and $l_2, l_3, \cdots, \geq$ [3. Since, for any connected graph

$$\gamma(G) \leq \frac{n}{2}$$

.

Therefore, we have

$$\gamma(SO(B_n^2)) \leq \frac{O(B_n^2)}{2}. \quad (33)$$

Also,

$$\gamma(SO'(B_n^2) \leq \frac{O(B_n^2)}{2}. \quad (34)$$

The edge set of $B_n^2(n \geq 4)$ can be partitioned into five disjoint sets $\varepsilon_{2,2}, \varepsilon_{2,3}$, $\varepsilon_{2,4}$, $\varepsilon_{3,3}$ and $\varepsilon_{3,4}$, where $\varepsilon(B_n^2(n \geq 4))$[$= \varepsilon_{2,2} \cup \varepsilon_{2,3} \cup$ [$\varepsilon_{2,4}$[$\cup$ [$\varepsilon_{3,3} \cup \varepsilon_{3,4}$. Further, $|\varepsilon_{2,2}| = 2$, $|\varepsilon_{2,3}| = 2m$, $|\varepsilon_{2,4}| = 2$, $|\varepsilon_{3,3}| =$ that $|\varepsilon(B_n^2(n \geq 3))| = |\varepsilon_{2,2}| + |\varepsilon_{2,3}|$[$+|\varepsilon_{2,4}|$[$+$[$|\varepsilon_{3,3}| + |\varepsilon_{3,4}|$. Thus, employing equations (1)-(2) and (33)-(34) we get the required result.

Theorem 16 *Let T_p be a triangular benzenoid where p shows the number of hexagons in the base graph and total number of hexagons in T_p is $\frac{p(p+1)}{2}$. Then*

$$SO(T_p) \leq \frac{O(T_p)}{2} + 6\sqrt{13}(p - 1) + \sqrt{8}(\frac{3p(p-1)}{2}) + 6\sqrt{8}$$

$$SO'(T_p) \leq \frac{O(T_p)}{2} + 36(p - 1) + \frac{27p(p-1)}{2}$$

Proof. Let T_p be a triangular benzenoid where p shows the number of hexagons in the base graph and total number of hexagons in T_p is $\frac{p(p+1)}{2}$. Since, for any connected graph

$$\gamma(G) \leq \frac{n}{2}$$

.

Therefore, we have

$$\gamma(SO(T_p)) \leq \frac{O(T_p)}{2}. \quad (35)$$

Also,

$$\gamma(SO'(T_p) \leq \frac{O(T_p)}{2}. \quad (36)$$

The edge set of T_p can be partitioned into three disjoint sets $\varepsilon_{2,2}, \varepsilon_{2,3}$ and $\varepsilon_{3,3}$ where $\varepsilon(T_p) = \varepsilon_{2,2}[\cup \varepsilon_{2,3} \cup \varepsilon_{3,3}$. Further, $|\varepsilon_{2,2}|[= 6$, $|\varepsilon_{2,3}| = [6(p-1)$ and $|\varepsilon_{3,3}| = \frac{3p(p-1)}{2}$. Such that $|\varepsilon(T_p)| = |\varepsilon_{2,2}| + |\varepsilon_{2,3}| + |\varepsilon_{3,3}|$. Thus, employing equations (1)-(2) and (35)-(36) we get the required result.

Theorem 17 *Let X_p be a benzenoid hourglass. Then*

$$SO(X_p) \leq \frac{O(X_p)}{2} + 4\sqrt{13}(3p-4) + \sqrt{18}(3p^2-3p+4) + 8\sqrt{8}$$
$$SO(X_p) \leq \frac{O(X_p)}{2} + 24(3p-4) + 9(3p^2-3p+4) + 32$$

Proof. Let X_p be a benzenoid hourglass. Since, for any connected graph

$$\gamma(G) \leq \frac{n}{2}$$

.

Therefore, we have

$$\gamma(SO(X_p)) \leq \frac{O(X_p)}{2}. \quad (37)$$

Also,

$$\gamma(SO'(X_p) \leq \frac{O(X_p)}{2}. \quad (38)$$

The edge set of X_p can be partitioned into three disjoint sets $\varepsilon_{2,2}$, $\varepsilon_{2,3}$ and $\varepsilon_{3,3}$ where $\varepsilon(X_p) = \varepsilon_{2,2} \cup \varepsilon_{2,3}[\cup [\varepsilon_{3,3}$. Further, $|\varepsilon_{2,2}|[rgb]1.00,1.00,1.00i = [8$, $|\varepsilon_{2,3}| = 4(3p-4)$ and $|\varepsilon_{3,3}| = 3p^2-3p+4$. Such that $|\varepsilon(X_p)| = |\varepsilon_{2,2}| + |\varepsilon_{2,3}|[r + |\varepsilon_{3,3}|$. Thus, with this background by employing equations (1)-(2) and (37)-(38), we get the required results.

Theorem 18 *Let $B_{p,q}$ be denote a jagged rectangle benzenoid system for all $p, q \in [N-1$. Then*

$$SO(B_{p,q}) \leq \frac{O(B_{p,q})}{2} + \sqrt{8}(2q+4) + \sqrt{13}(4p+4q-4) + \sqrt{18}(6pq+p-5q-4)$$

$$SO'(B_{p,q}) \leq \frac{O(B_{p,q})}{2} + 4(2q+4) + 6(4p+4q-4) + 9(6pq+p-5q-4)$$

Proof. Let $B_{p,q}$ be denote a jagged rectangle benzenoid system for all $p,\ q\ \in\ N-1$. Since, for any connected graph

$$\gamma(G) \leq \frac{n}{2}$$

.

Therefore, we have

$$\gamma(SO(B_{p,q})) \leq \frac{O(B_{p,q})}{2}. \qquad (39)$$

Also,

$$\gamma(SO'(B_{p,q}) \leq \frac{O(B_{p,q})}{2}. \qquad (40)$$

The edge set of $B_{p,q}$ can be partitioned into three disjoint sets $\varepsilon_{2,2}$, $\varepsilon_{2,3}$ and $\varepsilon_{3,3}$ where $\varepsilon(B_{p,q}) = \varepsilon_{2,2} \cup \varepsilon_{2,3} \cup \varepsilon_{3,3}$. Further, $|\varepsilon_{2,2}| = 2q+4$, $|\varepsilon_{2,3}| = 4p+4q-4$ and $|\varepsilon_{3,3}| = 6pq+p-5q-4$. Such that $|\varepsilon(B_{p,q})| = |\varepsilon_{2,2}| + |\varepsilon_{2,3}| + |\varepsilon_{3,3}|$. Thus, employing equations (1)-(2) and (39)-(40) we get the required result.

Conclusion: In this paper we have initiated the study of new topological indices and they are called invariants of Sombor index. The correlation of Sombor index with other its variants shows that these Sombor type invariants have equal potential like Sombor index. Finally, we have obtained bounds forthe set of nanostructures as well as dendrimers in terms of domination number and Sombor index.

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