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On topological properties of boron triangular sheet $BTS(m,n)$, borophene chain $B_{36}(n)$ and melem chain $MC(n)$ nanostructures

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Abstract. Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant. In QSAR/QSPR study, physico-chemical properties and topological indices such as Randić, atom-bond connectivity (ABC) and geometric-arithmetic (GA) index are used to predict the bioactivity of chemical compounds. Graph theory has found a considerable use in this area of research. In this paper, we study and derive analytical closed results of general Randić index $R_\alpha(G)$ with $\alpha = 1, \frac{1}{2}, -1, -\frac{1}{2}$, for boron triangular sheet $BTS(m,n)$, borophene chain of $B_{36}(n)$ and melem chain $MC(n)$. We also compute the general first Zagreb, ABC, GA, ABC_4 and GA_5 indices of sheet and chains for the first time and give closed formulas of these degree based indices.

Keywords: general Randić index, atom-bond connectivity (ABC) index, geometric-arithmetic (GA) index, boron triangular, borophene, melem
Mathematics Subject Classification (2010): 05C09.

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1 Introduction and preliminary results

Graph theory has provided chemist with a variety of useful tools, such as topological indices. Molecules and molecular compounds are often modeled by molecular graph. A molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory, whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. *Cheminformatics* is new subject which is a combination of chemistry, mathematics and information science. It studies Quantitative structure-activity (QSAR) and structure-property (QSPR) relationships that are used to predict the biological activities and properties of chemical compounds. In the QSAR /QSPR study, physico-chemical properties and topological indices such as Wiener index, Szeged index, Randić index, Zagreb indices and ABC index are used to predict bioactivity of the chemical compounds.

A graph can be recognized by a numeric number, a polynomial, a sequence of numbers or a matrix. A topological index is a numeric quantity associated with a graph which characterize the topology of graph and is invariant under graph automorphism. There are some major classes of topological indices such as distance based topological indices, degree based topological indices and counting related polynomials and indices of graphs. Among these classes degree based topological indices are of great importance and play a vital role in chemical graph theory and particularly in chemistry. In more precise way, a topological index $Top(G)$ of a graph, is a number with the property that for every graph H isomorphic to G, $Top(H) = Top(G)$. The concept of topological indices came from Wiener [24] while he was working on boiling point of paraffin, named this index as *path number*. Later on, the path number was renamed as *Wiener index* [5].

In this article, G is considered to be network with vertex set $V(G)$ and edge set $E(G)$, $deg(u)$ is the degree of vertex $u \in V(G)$ and $S_u = \sum_{v \in N_G(u)} deg(v)$ where $N_G(u) = \{v \in V(G) \mid uv \in E(G)\}$. The notations used in this article are mainly taken from books [6,10].

Let G be a graph. Then the Wiener index of G is defined as

$$W(G) = \frac{1}{2} \sum_{(u,v)} d(u,v), \tag{1}$$

where (u,v) is any ordered pair of vertices in G and $d(u,v)$ is $u - v$ geodesic.

The very first and oldest degree based topological index is *Randić* index [20] denoted by $R_{-\frac{1}{2}}(G)$ and introduced by Milan Randić and defined as

$$R_{-\frac{1}{2}}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{deg(u)deg(v)}}. \tag{2}$$

The general Randić index $R_\alpha(G)$ is the sum of $(deg(u)deg(v))^\alpha$ over all edges $e = uv \in E(G)$ defined as

$$R_\alpha(G) = \sum_{uv \in E(G)} (deg(u)deg(v))^\alpha \ \text{ for } \ \alpha = 1, \frac{1}{2}, -1, -\frac{1}{2}. \tag{3}$$

An important topological index introduced by Ivan Gutman and Trinajstić is the *Zagreb* index denoted by $M_1(G)$ and defined as

$$M_1(G) = \sum_{uv \in E(G)} (deg(u) + deg(v)). \tag{4}$$

One of the well-known degree based topological index is *atom-bond connectivity* (ABC) index introduced by Estrada *et al.* in [7] and defined as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{deg(u) + deg(v) - 2}{deg(u)deg(v)}}. \tag{5}$$

Another well-known connectivity topological descriptor is *geometric-arithmetic* (GA) index which was introduced by Vukičević *et al.* in [腳evi膰?,腳evi膰] and defined as

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{deg(u)deg(v)}}{(deg(u) + deg(v))}. \tag{6}$$

Only ABC_4 and GA_5 indices can be computed if we are able to find the edge partition of these interconnection networks based on sum of the degrees of end vertices of each edge in these graphs. The fourth version of ABC index is introduced by Ghorbani *et al.* [8] and defined as

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}. \tag{7}$$

Recently fifth version of GA index is proposed by Graovac *et al.* [9] and defined as

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_u S_v}}{(S_u + S_v)}. \tag{8}$$

The general Randić index for $\alpha = 1$ is the second Zagreb index for any graph G.

2 Main results

We study the general Randić, first Zagreb, ABC, GA, ABC_4 and GA_5 indices and give closed formulae of these indices for boron triangular sheet $BTS(m,n)$, borophene chain of $B_{36}(n)$ and melem chain $MC(n)$. Imran *et al.* studied various degree based topological indices for various networks like silicates, hexagonal, honeycomb and oxide in [12]. Nowadays there is an extensive research activity on ABC and GA indices and their variants, for further study of topological indices of various graph families see, [1–4, 13–19, 21, 22].

2.1 Results for $BTS(m,n)$, $B_{36}(n)$ and $MC(n)$ nanostructures

In this paper, we calculate certain degree based topological indices of boron triangular sheet $BTS(m,n)$, borophene chain of $B_{36}(N)$ and melem chain $MC(n)$ nanostructures. We compute general Randić $R_\alpha(G)$ with $\alpha = \{1, -1, \frac{1}{2}, -\frac{1}{2}\}$, ABC, GA, ABC_4 and GA_5 indices for $BTS(m,n)$, $B_{36}(n)$ and $MC(n)$ nanostructures.

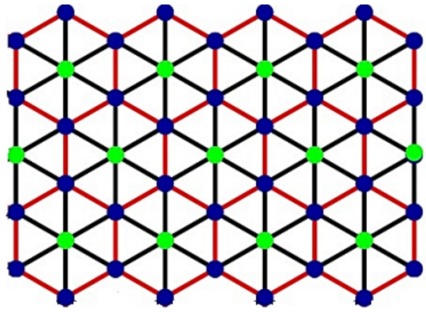

Figure 1. Boron triangular sheet (BTS(4, 4))).

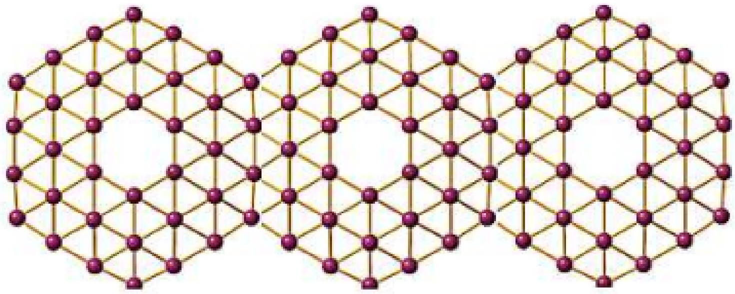

Figure 2. Borophene chain (B_{36}(n)(3)).

Theorem 2.1. *Consider the boron triangular sheet $BTS(m,n)$ for $m = n \geq 3$. Then*

$$R_\alpha(BTS(m,n)) = \begin{cases} -2(7m - 108mn + 7(2+n)), & \alpha = 1; \\ 12 + 8\sqrt{3} + 4(-4+m+n)+ \\ (4\sqrt{6} + 2\sqrt{15} + 3\sqrt{30})(-2+m+n)+ \\ 3\sqrt{2}(4+m+n) - 36(-1+m-mn+n), & \alpha = \frac{1}{2}; \\ \frac{1}{720}(204 + 193m + 120mn + 193n), & \alpha = -1; \\ \frac{1}{60}(80 + 40\sqrt{3} + 15(-4+m+n)+ \\ (10\sqrt{6} + 8\sqrt{5} + 6\sqrt{30})(-2+m+n)+ \\ 10\sqrt{2}(4+m+n) - 60(-1+m-mn+n)), & \alpha = -\frac{1}{2}. \end{cases}$$

Proof. Let $G \cong BTS(m,n)$ be the boron triangular sheet. The boron triangular sheet $BTS(m,n)$ has $m+n+4$ vertices of degree 3, $m+n-2$ vertices of degree 4, $m+n-2$ vertices of degree 5 and $2mn - m - n + 1$ vertices of degree 6. The edge set of $BTS(m,n)$ is divided into eight partitions based on the degree of end vertices. The first edge partition $E_1(BTS(m,n))$ contains 4 edges uv, where $deg(u) = deg(v) = 3$. The second edge partition $E_2(BTS(m,n))$

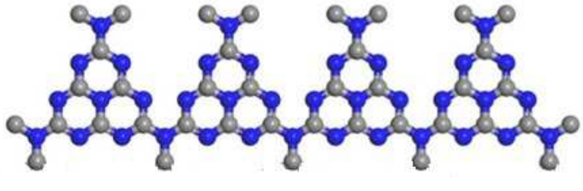

Figure 3. Melem chain (MC(4)).

(d_u,d_v), $(uv \in E(G))$	Number of edges
(3,3)	4
(3,4)	4
(3,5)	$2(m+n-2)$
(3,6)	$m+n+4$
(4,4)	$m+n-4$
(4,6)	$2(m+n-2)$
(5,6)	$3(m+n-2)$
(6,6)	$6(mn-(m+n)+1)$

Table 1. Edge partition of boron triangular sheet $BTS(m,n)$ based on degrees of end vertices of each edge.

contains 4 edges uv, where $deg(u)=3$ and $deg(v)=4$. The third edge partition $E_3(BTS(m,n))$ contains $2m+2n-4$ edges uv, where $deg(u)=3$ and $deg(v)=5$. The fourth edge partition $E_4(BTS(m,n))$ contains $m+n+4$ edges uv, where $deg(u)=3$ and $deg(v)=6$. The fifth edge partition $E_5(BTS(m,n))$ contains $m+n-4$ edges uv, where $deg(u)=deg(v)=4$. The sixth edge partition $E_6(BTS(m,n))$ contains $2m+2n-4$ edges uv, where $deg(u)=4$ and $deg(v)=6$. The seventh edge partition $E_7(BTS(m,n))$ contains $3m+3n-6$ edges uv, where $deg(u)=5$ and $deg(v)=6$ and the eighth edge partition $E_8(BTS(m,n))$ contains $6mn-6m-6n+6$ edges uv, where $deg(u)=deg(v)=6$. Table 1 shows such an edge partition of $BTS(m,n)$. Thus from (3) it follows that

$$R_\alpha(G)=\sum_{uv\in E(G)}(deg(u)\cdot deg(v))^\alpha.$$

Now, we apply the formula of $R_\alpha(G)$ for $\alpha=1$

$$R_1(G)=\sum_{j=1}^{8}\sum_{uv\in E_j(G)} deg(u)\cdot deg(v).$$

By using edge partition given in Table 1, we get

$$\begin{aligned}R_1(G) &= 9|E_1(BTS(m,n))|+12|E_2(BTS(m,n))|+15|E_3(BTS(m,n))|+18|E_4(BTS(m,n))|\\ &\quad +16|E_5(BTS(m,n))|+24|E_6(BTS(m,n))|+30|E_7(BTS(m,n))|+36|E_8(BTS(m,n))|\\ &= -2(7m-108mn+7(2+n)).\end{aligned}$$

We apply the formula of $R_\alpha(G)$ for $\alpha=\frac{1}{2}$

$$R_{\frac{1}{2}}(G)=\sum_{j=1}^{8}\sum_{uv\in E_j(G)}\sqrt{deg(u)\cdot deg(v)}.$$

By using edge partition given in Table 1, we get

$$\begin{aligned}
R_{\frac{1}{2}}(G) &= 3|E_1(BTS(m,n))| + 2\sqrt{3}|E_2(BTS(m,n))| + \sqrt{15}|E_3(BTS(m,n))| \\
&+ 3\sqrt{2}|E_4(BTS(m,n))| + 4|E_5(BTS(m,n))| + 2\sqrt{6}|E_6(BTS(m,n))| \\
&+ \sqrt{30}|E_7(BTS(m,n))| + 6|E_8(BTS(m,n))| \\
&= 12 + 8\sqrt{3} + 4(-4+m+n) + (4\sqrt{6} + 2\sqrt{15} + 3\sqrt{30})(-2+m+n) \\
&+ 3\sqrt{2}(4+m+n) - 36(-1+m-mn+n).
\end{aligned}$$

We apply the formula of $R_\alpha(G)$ for $\alpha = -1$. Then we have

$$\begin{aligned}
R_{-1}(G) &= \sum_{j=1}^{8} \sum_{uv \in E_j(G)} \frac{1}{deg(u) \cdot deg(v)} \\
&= \frac{1}{9}|E_1(BTS(m,n))| + \frac{1}{12}|E_2(BTS(m,n))| + \frac{1}{15}|E_3(BTS(m,n))| \\
&+ \frac{1}{18}|E_4(BTS(m,n))| + \frac{1}{16}|E_5(BTS(m,n))| + \frac{1}{24}|E_6(BTS(m,n))| \\
&+ \frac{1}{30}|E_7(BTS(m,n))| + \frac{1}{36}|E_8(BTS(m,n))| \\
&= \frac{1}{720}(204 + 193m + 120mn + 193n).
\end{aligned}$$

We apply the formula of $R_\alpha(G)$ for $\alpha = -\frac{1}{2}$. Then we have

$$\begin{aligned}
R_{-\frac{1}{2}}(G) &= \sum_{j=1}^{8} \sum_{uv \in E_j(G)} \frac{1}{\sqrt{deg(u) \cdot deg(v)}} \\
&= \frac{1}{3}|E_1(BTS(m,n))| + \frac{\sqrt{3}}{6}|E_2(BTS(m,n))| + \frac{1}{\sqrt{15}}|E_3(BTS(m,n))| \\
&+ \frac{\sqrt{2}}{6}|E_4(BTS(m,n))| + \frac{1}{4}|E_5(BTS(m,n))| + \frac{\sqrt{6}}{12}|E_6(BTS(m,n))| \\
&+ \frac{1}{\sqrt{30}}|E_7(BTS(m,n))| + \frac{1}{6}|E_8(BTS(m,n))| \\
&= \frac{1}{60}(80 + 40\sqrt{3} + 15(-4+m+n) + (10\sqrt{6} + 8\sqrt{5} + 6\sqrt{30})(-2+m+n) \\
&+ 10\sqrt{2}(4+m+n) - 60(-1+m-mn+n)).
\end{aligned}$$

□

In the following, we compute first Zagreb index of boron triangular sheet $BTS(m,n)$.

Theorem 2.2. *For boron triangular sheet $G \cong BTS(m,n)$ for $m = n \geq 3$, We have*

$$M_1(BTS(m,n)) = 2(-5 + 7m + 36mn + 7n).$$

Proof. Let G be the boron triangular sheet $BTS(m,n)$. By using edge partition from Table 1, the result follows. From (4) we have

$$
\begin{aligned}
M_1(BTS(m,n)) &= \sum_{uv\in E(G)} (deg(u)+deg(v)) = \sum_{j=1}^{8} \sum_{uv\in E_j(G)} (deg(u)+deg(v)) \\
&= 6|E_1(BTS(m,n))| + 7|E_2(BTS(m,n))| + 8|E_3(BTS(m,n))| \\
&+ 9|E_4(BTS(m,n))| + 8|E_5(BTS(m,n))| + 10|E_6(BTS(m,n))| \\
&+ 11|E_7(BTS(m,n))| + 12|E_8(BTS(m,n))|.
\end{aligned}
$$

By doing some calculation, we get $M_1(BTS(m,n)) = 2(-5+7m+36mn+7n)$. □

Now, we compute ABC and GA indices of boron triangular sheet $BTS(m,n)$.

Theorem 2.3. *Let $G \cong BTS(m,n)$ be the boron triangular sheet, for $m = n \geq 3$, then*

$$
\begin{aligned}
ABC(G) &= \frac{1}{60}(160 + 40\sqrt{15} + 15\sqrt{6}(-4+m+n) \\
&+ (40\sqrt{3} + 24\sqrt{10} + 18\sqrt{30})(-2+m+n) \\
&+ 10\sqrt{14}(4+m+n) - 60\sqrt{10}(-1+m-mn+n)), \\
GA(G) &= 6 + \frac{16}{7}\sqrt{3} - 5m + 6mn - 5n \\
&+ (\frac{4}{5}\sqrt{6} + \frac{\sqrt{15}}{2} + \frac{6}{11}\sqrt{30}(-2+m+n) + \frac{2}{3}\sqrt{2}(4+m+n)).
\end{aligned}
$$

Proof. By using edge partition given in Table 1, we get the result. From (5) it follows that

$$
\begin{aligned}
ABC(G) &= \sum_{uv\in E(G)} \sqrt{\frac{deg(u)+deg(v)-2}{deg(u)\cdot deg(v)}} = \sum_{j=1}^{8} \sum_{uv\in E_j(G)} \sqrt{\frac{deg(u)+deg(v)-2}{deg(u)\cdot deg(v)}} \\
&= \frac{2}{3}|E_1(BTS(m,n))| + \frac{\sqrt{15}}{6}|E_2(BTS(m,n))| + \frac{\sqrt{10}}{5}|E_3(BTS(m,n))| \\
&+ \frac{\sqrt{14}}{6}|E_4(BTS(m,n))| + \frac{\sqrt{6}}{4}|E_5(BTS(m,n))| + \frac{\sqrt{3}}{3}|E_6(BTS(m,n))| \\
&+ \frac{\sqrt{30}}{10}|E_7(BTS(m,n))| + \frac{\sqrt{10}}{6}|E_8(BTS(m,n))|.
\end{aligned}
$$

By doing some calculation, we get

$$
\begin{aligned}
ABC(G) &= \frac{1}{60}\big(160 + 40\sqrt{15} + 15\sqrt{6}(-4+m+n) \\
&+ (40\sqrt{3} + 24\sqrt{10} + 18\sqrt{30})(-2+m+n) + 10\sqrt{14}(4+m+n) \\
&- 60\sqrt{10}(-1+m-mn+n)\big),
\end{aligned}
$$

and from (6) we get

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{deg(u)deg(v)}}{(deg(u)+deg(v))} \sum_{j=1}^{8} \sum_{uv\in E_j(G)} \frac{2\sqrt{deg(u)deg(v)}}{(deg(u)+deg(v))}.$$

Then we have

$$\begin{aligned} GA(G) = {} & |E_1(BTS(m,n))| + \frac{4}{7}\sqrt{3}|E_2(BTS(m,n))| + \frac{\sqrt{15}}{4}|E_3(BTS(m,n))| \\ & + \frac{2}{3}\sqrt{2}|E_4(BTS(m,n))| + |E_5(BTS(m,n))| + \frac{2}{5}\sqrt{6}|E_6(BTS(m,n))| \\ & + \frac{2}{11}\sqrt{30}|E_7(BTS(m,n))| + |E_8(BTS(m,n))|. \end{aligned}$$

By doing some calculation, we get

$$\begin{aligned} GA(G) = {} & 6 + \frac{16}{7}\sqrt{3} - 5m + 6mn - 5n \\ & + (\frac{4}{5}\sqrt{6} + \frac{\sqrt{15}}{2} + \frac{6}{11}\sqrt{30}(-2+m+n) + \frac{2}{3}\sqrt{2}(4+m+n)). \end{aligned}$$

□

Now, we compute ABC_4 and GA_5 indices of boron triangular sheet $BTS(m,n)$. Let us consider an edge partition based on degree sum of neighbors of end vertices. Then the edge set $E(BTS(m,n))$ can be divided into twenty four edge partitions $E_j(BTS(m,n)), 9 \leq j \leq 32$, where the edge partition $E_9(BTS(m,n))$ contains 4 edges uv with $S_u = 13$ and $S_v = 14$, the edge partition $E_{10}(BTS(m,n))$ contains 4 edges uv with $S_u = 13$ and $S_v = 19$, the edge partition $E_{11}(BTS(m,n))$ contains 4 edges uv with $S_u = 13$ and $S_v = 27$, the edge partition $E_{12}(BTS(m,n))$ contains 4 edges uv with $S_u = 14$ and $S_v = 24$, the edge partition $E_{13}(BTS(m,n))$ contains 4 edges uv with $S_u = 14$ and $S_v = 27$, the edge partition $E_{14}(BTS(m,n))$ contains $2m+2n-8$ edges uv with $S_u = 16$ and $S_v = 24$, the edge partition $E_{15}(BTS(m,n))$ contains $m+n-4$ edges uv with $S_u = 16$ and $S_v = 31$, $E_{16}(BTS(m,n))$ contains 4 edges uv with $S_u = 19$ and $S_v = 20$, $E_{17}(BTS(m,n))$ contains 4 edges uv with $S_u = 19$ and $S_v = 27$, $E_{18}(BTS(m,n))$ contains 4 edges uv with $S_u = 19$ and $S_v = 32$, $E_{19}(BTS(m,n))$ contains $m+n-8$ edges uv with $S_u = S_v = 20$, $E_{20}(BTS(m,n))$ contains $2m+2n-12$ edges uv with $S_u = 20$ and $S_v = 32$, $E_{21}(BTS(m,n))$ contains 4 edges uv with $S_u = 24$ and $S_v = 27$, $E_{22}(BTS(m,n))$ contains $2m+2n-8$ edges uv with $S_u = 24$ and $S_v = 31$, $E_{23}(BTS(m,n))$ contains $m+n-2$ edges uv with $S_u = 24$ and $S_v = 35$, $E_{24}(BTS(m,n))$ contains 4 edges uv with $S_u = 27$ and $S_v = 32$, $E_{25}(BTS(m,n))$ contains 4 edges uv with $S_u = 27$ and $S_v = 35$, $E_{26}(BTS(m,n))$ contains $2m+2n-8$ edges uv with $S_u = 31$ and $S_v = 35$, $E_{27}(BTS(m,n))$ contains $m+n-4$ edges uv with $S_u = 31$ and $S_v = 36$, $E_{28}(BTS(m,n))$ contains $m+n-6$ edges uv with $S_u = S_v = 32$, $E_{29}(BTS(m,n))$ contains 4 edges uv with $S_u = 32$ and $S_v = 35$, $E_{30}(BTS(m,n))$ contains $2m+2n-12$ edges uv with $S_u = 32$ and $S_v = 36$, $E_{31}(BTS(m,n))$ contains $3m+3n-10$ edges uv with $S_u = 35$ and $S_v = 36$ and $E_{32}(BTS(m,n))$ contains $6mn-15m-15n+34$ edges uv with $S_u = S_v = 36$.

Theorem 2.4. *Let $G \cong BTS(m,n)$ be the boron triangular sheet, for $m = n \geq 5$, then*

$$\begin{aligned}
ABC_4(G) &= 10\sqrt{\frac{2}{91}} + 4\sqrt{\frac{30}{247}} + \frac{8}{3}\sqrt{\frac{11}{57}} + 2\sqrt{\frac{37}{95}} + 2\sqrt{\frac{3}{7}} + \sqrt{\frac{13}{14}} + \frac{7}{9}\sqrt{2} + \frac{2}{3}\sqrt{\frac{26}{7}} \\
&+ \frac{8}{3\sqrt{7}} + \frac{1}{3}\sqrt{\frac{19}{2}} + \frac{7}{\sqrt{38}} + \frac{152}{3\sqrt{39}} + \frac{1}{18}\sqrt{\frac{35}{2}}(34 - 15m + 6mn - 15n) \\
&+ \frac{1}{10}\sqrt{\frac{19}{2}}(-8 + m + n) + (\frac{1}{4}\sqrt{\frac{11}{3}} + \frac{1}{4}\sqrt{5} + \frac{1}{16}\sqrt{\frac{31}{2}})(-6 + m + n) \\
&+ (\frac{3}{4}\sqrt{\frac{5}{31}} + \sqrt{\frac{53}{186}} + \frac{1}{6}\sqrt{\frac{65}{31}} + \frac{1}{4}\sqrt{\frac{19}{3}} + \frac{16}{\sqrt{1085}})(-4 + m + n) \\
&+ \frac{1}{2}\sqrt{\frac{19}{70}}(-2 + m + n) + \frac{1}{2}\sqrt{\frac{23}{105}}(-10 + 3m + 3n), \\
GA_5(G) &= 20 + \frac{48}{17}\sqrt{2} + \frac{96}{59}\sqrt{6} + \frac{16}{19}\sqrt{21} + \frac{32}{51}\sqrt{38} + \frac{3}{5}\sqrt{39} + \frac{24}{41}\sqrt{42} \\
&+ \frac{12}{23}\sqrt{57} + \frac{32}{67}\sqrt{70} + \frac{16}{39}\sqrt{95} + \frac{12}{31}\sqrt{105} + \frac{8}{27}\sqrt{182} + \frac{1}{4}\sqrt{247} \\
&- 13m + 6mn - 13n + (\frac{24}{17}\sqrt{2} + \frac{8}{13}\sqrt{10})(-6 + m + n) \\
&+ (\frac{4}{5}\sqrt{6} + \frac{1100}{3149}\sqrt{31} + \frac{8}{55}\sqrt{186} + \frac{2}{33}\sqrt{1085})(-4 + m + n) \\
&+ \frac{4}{59}\sqrt{210}(-2 + m + n) + \frac{12}{71}\sqrt{35}(-10 + 3m + 3n).
\end{aligned}$$

Proof. By using edge partition given in Table 2, we get the result. From (7) it follows that

$$\begin{aligned}
ABC_4(G) &= \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}} = \sum_{j=9}^{32} \sum_{uv \in E_j(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}} \\
&= \frac{5}{\sqrt{182}}|E_9(BTS(m,n))| + \sqrt{\frac{30}{247}}|E_{10}(BTS(m,n))| + \frac{1}{3}\sqrt{\frac{38}{39}}|E_{11}(BTS(m,n))| \\
&+ \frac{\sqrt{21}}{14}|E_{12}(BTS(m,n))| + \frac{\sqrt{182}}{42}|E_{13}(BTS(m,n))| + \frac{\sqrt{57}}{24}|E_{14}(BTS(m,n))| \\
&+ \frac{3}{4}\sqrt{\frac{5}{31}}|E_{15}(BTS(m,n))| + \frac{1}{2}\sqrt{\frac{37}{95}}|E_{16}(BTS(m,n))| + \frac{2}{3}\sqrt{\frac{11}{57}}|E_{17}(BTS(m,n))| \\
&+ \frac{1}{4}\frac{7}{\sqrt{38}}|E_{18}(BTS(m,n))| + \frac{\sqrt{38}}{20}|E_{19}(BTS(m,n))| + \frac{\sqrt{5}}{8}|E_{20}(BTS(m,n))| \\
&+ \frac{7}{36}\sqrt{2}|E_{21}(BTS(m,n))| + \frac{1}{2}\sqrt{\frac{53}{186}}|E_{22}(BTS(m,n))| + \frac{3}{2}\sqrt{\frac{6}{210}}|E_{23}(BTS(m,n))| \\
&+ \frac{\sqrt{38}}{24}|E_{24}(BTS(m,n))| + \frac{2}{21}\sqrt{7}|E_{25}(BTS(m,n))| + \frac{8}{\sqrt{1085}}|E_{26}(BTS(m,n))| \\
&+ \frac{1}{6}\sqrt{\frac{65}{31}}|E_{27}(BTS(m,n))| + \frac{\sqrt{62}}{32}|E_{28}(BTS(m,n))| + \frac{\sqrt{182}}{56}|E_{29}(BTS(m,n))|
\end{aligned}$$

$$+ \frac{\sqrt{33}}{24}|E_{30}(BTS(m,n))| + \frac{1}{6}\sqrt{\frac{69}{35}}|E_{31}(BTS(m,n))| + \frac{\sqrt{70}}{36}|E_{32}(BTS(m,n))|.$$

Thus, we have

$$\begin{aligned} ABC_4(G) &= 10\sqrt{\frac{2}{91}} + 4\sqrt{\frac{30}{247}} + \frac{8}{3}\sqrt{\frac{11}{57}} + 2\sqrt{\frac{37}{95}} + 2\sqrt{\frac{3}{7}} + \sqrt{\frac{13}{14}} + \frac{7}{9}\sqrt{2} + \frac{2}{3}\sqrt{\frac{26}{7}} \\ &+ \frac{8}{3\sqrt{7}} + \frac{1}{3}\sqrt{\frac{19}{2}} + \frac{7}{\sqrt{38}} + \frac{152}{3\sqrt{39}} + \frac{1}{18}\sqrt{\frac{35}{2}}(34 - 15m + 6mn - 15n) \\ &+ \frac{1}{10}\sqrt{\frac{19}{2}}(-8 + m + n) + (\frac{1}{4}\sqrt{\frac{11}{3}} + \frac{1}{4}\sqrt{5} + \frac{1}{16}\sqrt{\frac{31}{2}})(-6 + m + n) \\ &+ (\frac{3}{4}\sqrt{\frac{5}{31}} + \sqrt{\frac{53}{186}} + \frac{1}{6}\sqrt{\frac{65}{31}} + \frac{1}{4}\sqrt{\frac{19}{3}} + \frac{16}{\sqrt{1085}})(-4 + m + n) \\ &+ \frac{1}{2}\sqrt{\frac{19}{70}}(-2 + m + n) + \frac{1}{2}\sqrt{\frac{23}{105}}(-10 + 3m + 3n). \end{aligned}$$

From (8) we get

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_u S_v}}{(S_u + S_v)} = \sum_{j=9}^{32} \sum_{uv \in E_j(G)} \frac{2\sqrt{S_u S_v}}{(S_u + S_v)}.$$

Then,

$$\begin{aligned} GA_5(G) &= 2\frac{\sqrt{182}}{27}|E_9(BTS(m,n))| + \frac{\sqrt{247}}{16}|E_{10}(BTS(m,n))| + 3\frac{\sqrt{39}}{20}|E_{11}(BTS(m,n))| \\ &+ 4\frac{\sqrt{21}}{19}|E_{12}(BTS(m,n))| + 6\frac{\sqrt{42}}{41}|E_{13}(BTS(m,n))| + 2\frac{\sqrt{6}}{5}|E_{14}(BTS(m,n))| \\ &+ 8\frac{\sqrt{31}}{47}|E_{15}(BTS(m,n))| + 4\frac{\sqrt{95}}{39}|E_{16}(BTS(m,n))| + 3\frac{\sqrt{57}}{23}|E_{17}(BTS(m,n))| \\ &+ 8\frac{\sqrt{38}}{51}|E_{18}(BTS(m,n))| + |E_{19}(BTS(m,n))| + 4\frac{\sqrt{10}}{13}|E_{20}(BTS(m,n))| \\ &+ 12\frac{\sqrt{2}}{17}|E_{21}(BTS(m,n))| + 4\frac{\sqrt{186}}{55}|E_{22}(BTS(m,n))| + 4\frac{\sqrt{210}}{59}|E_{23}(BTS(m,n))| \\ &+ 24\frac{\sqrt{6}}{59}|E_{24}(BTS(m,n))| + 3\frac{\sqrt{105}}{31}|E_{25}(BTS(m,n))| + \frac{\sqrt{1085}}{33}|E_{26}(BTS(m,n))| \\ &+ 12\frac{\sqrt{31}}{67}|E_{27}(BTS(m,n))| + |E_{28}(BTS(m,n))| + 8\frac{\sqrt{70}}{67}|E_{29}(BTS(m,n))| \\ &+ 12\frac{\sqrt{2}}{17}|E_{30}(BTS(m,n))| + 12\frac{\sqrt{35}}{71}|E_{31}(BTS(m,n))| + |E_{32}(BTS(m,n))|. \end{aligned}$$

Thus, we have

$$GA_5(G) = 20 + \frac{48}{17}\sqrt{2} + \frac{96}{59}\sqrt{6} + \frac{16}{19}\sqrt{21} + \frac{32}{51}\sqrt{38} + \frac{3}{5}\sqrt{39} + \frac{24}{41}\sqrt{42} + \frac{12}{23}\sqrt{57} + \frac{32}{67}\sqrt{70}$$
$$+ \frac{16}{39}\sqrt{95} + \frac{12}{31}\sqrt{105} + \frac{8}{27}\sqrt{182} + \frac{1}{4}\sqrt{247} - 13m + 6mn - 13n$$
$$+ (\frac{24}{17}\sqrt{2} + \frac{8}{13}\sqrt{10})(-6 + m + n)$$
$$+ (\frac{4}{5}\sqrt{6} + \frac{1100}{3149}\sqrt{31} + \frac{8}{55}\sqrt{186} + \frac{2}{33}\sqrt{1085})(-4 + m + n)$$
$$+ \frac{4}{59}\sqrt{210}(-2 + m + n) + \frac{12}{71}\sqrt{35}(-10 + 3m + 3n).$$

□

Chemical engineers have determined that a unique arrangement of 36 boron-atoms in a flat disc with a hexagonal hole in the middle may be preferred building blocks for borophene. A 36-atom cluster of boron, left, arranged as a flat disc with a hexagonal hole in the middle, fix the theoretical requirements for making a one-atom-thick boron chain, right, a theoretical nanomaterial dubbed borophene. A borophene chain $B_{36}(n)$ for $n \geq 2$ has order $32n + 4$ and size $81n + 3$.

Now, we calculate certain degree based topological indices of borophene chain $B_{36}(n)$ of dimension n. In the coming theorems we compute general Randić index $R_\alpha(G)$ with $\alpha = \{1, -1, \frac{1}{2}, -\frac{1}{2}\}$, ABC, GA, ABC_4 and GA_5 of $B_{36}(n)$.

Theorem 2.5. *Consider the borophene chain $B_{36}(n)$ for $n \geq 2$. Then*

$$R_\alpha(B_{36}(n)) = \begin{cases} 6(-32 + 373n), & \alpha = 1; \\ 8 + 8\sqrt{5}(-1 + n) + 46n + (6\sqrt{2} + 8\sqrt{3})(2 + n) + & \\ 16\sqrt{6}(1 + 2n) + 6\sqrt{30}(-1 + 4n) + 18(-3 + 7n), & \alpha = \frac{1}{2}; \\ \frac{1}{1800}(1255 + 5732n), & \alpha = -1; \\ \frac{1}{30}(-30 + 20\sqrt{2} + 40\sqrt{3} - 12\sqrt{5} + 20\sqrt{6} - 6\sqrt{30} + & \\ (171 + 10\sqrt{2} + 20\sqrt{3} + 12\sqrt{3} + 40\sqrt{6} + 24\sqrt{30})n), & \alpha = -\frac{1}{2}. \end{cases}$$

Proof. Let G be the borophene chanin $B_{36}(n)$. The borophene chain $B_{36}(n)$ has $2n + 4$ vertices of degree 3, $8n + 4$ vertices of degree 4, $8n - 2$ vertices of degree 5 and $14n - 2$ vertices of degree 6. The edge set of $B_{36}(n)$ is divided into eight partitions based on the degree of end vertices. The first edge partition $E_1(B_{36}(n))$ contains $4n + 8$ edges uv, where $deg(u) = 3$ and $deg(v) = 4$. The second edge partition $E_2(B_{36}(n))$ contains $2n + 4$ edges uv, where $deg(u) = 3$ and $deg(v) = 6$. The third edge partition $E_3(B_{36}(n))$ contains $4n + 2$ edges uv, where $deg(u) = deg(v) = 4$. The forth edge partition $E_4(B_{36}(n))$ contains $4n - 4$ edges uv, where $deg(u) = 4$ and $deg(v) = 5$. The fifth edge partition $E_5(B_{36}(n))$ contains $16n + 8$ edges uv, where $deg(u) = 4$ and $deg(v) = 6$. The sixth edge partition $E_6(B_{36}(n))$ contains $6n$ edges uv, where $deg(u) = deg(v) = 5$. The seventh edge partition $E_7(B_{36}(n))$ contains $24n - 6$ edges

(S_u,S_v), $uv \in E(G)$	Number of edges	(S_u,S_v), $uv \in E(G)$	Number of edges
(13,14)	4	(24,27)	4
(13,19)	4	(24,31)	$2m+2n-8$
(13,27)	4	(24,35)	$m+n-2$
(14,24)	4	(27,32)	4
(14,27)	4	(27,35)	4
(16,24)	$2m+2n-8$	(31,35)	$2m+2n-8$
(16,31)	$m+n-4$	(31,36)	$m+n-4$
(19,20)	4	(32,32)	$m+n-6$
(19,27)	4	(32,35)	4
(19,32)	4	(32,36)	$2m+2n-12$
(20,20)	$m+n-8$	(35,36)	$3m+3n-10$
(20,32)	$2m+2n-12$	(36,36)	$6mn-15(m+n)+34$

Table 2. Edge partition of boron triangular sheet $BTS(m,n)$ based on degrees sum of end vertices of each edge.

(d_u,d_v), $uv \in E(G)$	Number of edges
(3,4)	$4n+8$
(3,6)	$2n+4$
(4,4)	$4n+2$
(4,5)	$4n-4$
(4,6)	$16n+8$
(5,5)	$6n$
(5,6)	$24n-6$
(6,6)	$21n-9$

Table 3. Edge partition of borophene chain $B_{36}(n)$ based on degrees of end vertices of each edge.

uv, where $deg(u)=5$ and $deg(v)=6$. The eight edge partition $E_8(B_{36}(n))$ contains $21n-9$ edges uv, where $deg(u)=deg(v)=6$. Table 3 shows such an edge partition of $B_{36}(n)$. Thus from (3) is follows that

$$R_\alpha(G)=\sum_{uv\in E(G)}(deg(u)deg(v))^\alpha.$$

Now we apply the formula of $R_\alpha(G)$ for $\alpha=1$

$$R_1(G)=\sum_{j=1}^{8}\sum_{uv\in E_j(G)}deg(u)\cdot deg(v).$$

By using edge partition given in Table 3, we get

$$\begin{aligned}R_1(G)&=12|E_1(B_{36}(n))|+18|E_2(B_{36}(n))|+16|E_3(B_{36}(n))|+20|E_4(B_{36}(n))|\\&+24|E_5(B_{36}(n))|+25|E_6(B_{36}(n))|+30|E_7(B_{36}(n))|+36|E_8(B_{36}(n))|.\end{aligned}$$

Then $R_1(G) = 6(-32 + 373n)$. We apply the formula of $R_\alpha(G)$ for $\alpha = \frac{1}{2}$

$$R_{\frac{1}{2}}(G) = \sum_{j=1}^{8} \sum_{uv \in E_j(G)} \sqrt{deg(u) \cdot deg(v)}.$$

By using edge partition given in Table 3, we get

$$\begin{aligned} R_{\frac{1}{2}}(G) &= 2\sqrt{3}|E_1(B_{36}(n))| + 3\sqrt{2}|E_2(B_{36}(n))| + 4|E_3(B_{36}(n))| + 2\sqrt{5}|E_4(B_{36}(n))| \\ &\quad + 2\sqrt{6}|E_5(B_{36}(n))| + 5|E_6(B_{36}(n))| + \sqrt{30}|E_7(B_{36}(n))| + 6|E_8(B_{36}(n))|. \end{aligned}$$

Then

$$\begin{aligned} R_{\frac{1}{2}}(G) &= 8 + 8\sqrt{5}(-1 + n) + 46n + (6\sqrt{2} + 8\sqrt{3})(2 + n) + 16\sqrt{6}(1 + 2n) \\ &\quad + 6\sqrt{30}(-1 + 4n) + 18(-3 + 7n). \end{aligned}$$

We apply the formula of $R_\alpha(G)$ for $\alpha = -1$

$$R_{-1}(G) = \sum_{j=1}^{8} \sum_{uv \in E_j(G)} \frac{1}{deg(u) \cdot deg(v)}.$$

We have

$$\begin{aligned} R_{-1}(G) &= \frac{1}{12}|E_1(B_{36}(n))| + \frac{1}{18}|E_2(B_{36}(n))| + \frac{1}{16}|E_3(B_{36}(n))| + \frac{1}{20}|E_4(B_{36}(n))| \\ &\quad + \frac{1}{24}|E_5(B_{36}(n))| + \frac{1}{25}|E_6(B_{36}(n))| + \frac{1}{30}|E_7(B_{36}(n))| + \frac{1}{36}|E_8(B_{36}(n))| \\ &= \frac{1}{1800}(1255 + 5732n). \end{aligned}$$

We apply the formula of $R_\alpha(G)$ for $\alpha = -\frac{1}{2}$

$$R_{-\frac{1}{2}}(G) = \sum_{j=1}^{8} \sum_{uv \in E_j(G)} \frac{1}{\sqrt{deg(u) \cdot deg(v)}}.$$

Thus

$$\begin{aligned} R_{-\frac{1}{2}}(G) &= \frac{\sqrt{3}}{6}|E_1(B_{36}(n))| + \frac{\sqrt{2}}{6}|E_2(B_{36}(n))| + \frac{1}{4}|E_3(B_{36}(n))| + \frac{\sqrt{5}}{10}|E_4(B_{36}(n))| \\ &\quad + \frac{\sqrt{6}}{12}|E_5(B_{36}(n))| + \frac{1}{5}|E_6(B_{36}(n))| + \frac{\sqrt{30}}{30}|E_7(B_{36}(n))| + \frac{1}{6}|E_8(B_{36}(n))| \\ &= \frac{1}{30}(-30 + 20\sqrt{2} + 40\sqrt{3} - 12\sqrt{5} + 20\sqrt{6} - 6\sqrt{30} \\ &\quad + (171 + 10\sqrt{2} + 20\sqrt{3} + 12\sqrt{3} + 40\sqrt{6} + 24\sqrt{30})n). \end{aligned}$$

□

In the following theorem, we compute first Zagreb index of borophene chain $B_{36}(n)$.

Theorem 2.6. *For borophene chain $G \cong B_{36}(n)$ for $n \geq 2$. Then*

$$M_1(B_{36}(n)) = -22 + 850n.$$

Proof. Let G be the borophene chain $B_{36}(n)$. By using edge partition from Table 3, the result follows. From (4) we have

$$M_1(B_{36}(n)) = \sum_{uv \in E(G)} (deg(u) + deg(v)) = \sum_{j=1}^{8} \sum_{uv \in E_j(G)} (deg(u) + deg(v)).$$

Then we have

$$\begin{aligned} M_1(B_{36}(n)) &= 7|E_1(B_{36}(n))| + 9|E_2(B_{36}(n))| + 8|E_3(B_{36}(n))| + 9|E_4(B_{36}(n))| \\ &+ 10|E_5(B_{36}(n))| + 10|E_6(B_{36}(n))| + 11|E_7(B_{36}(n))| + 12|E_8(B_{36}(n))|. \end{aligned}$$

By doing some calculation, we get $M_1(B_{36}(n)) = -22 + 850n$. □

Now, we compute ABC and GA indices of borophene chain $B_{36}(n)$.

Theorem 2.7. *Let $G \cong B_{36}(n)$ be the borophene chain, for $n \geq 2$, then*

$$\begin{aligned} ABC(G) &= \frac{1}{60}(24\sqrt{35}(-1+n) + 144\sqrt{2}n + (20\sqrt{14} + 40\sqrt{15})(2+n) \\ &+ (160\sqrt{3} + 30\sqrt{6})(1+2n) + 36\sqrt{30}(-1+4n) + 30\sqrt{10}(-3+7n)), \\ GA(G) &= -7 + \frac{16}{9}\sqrt{5}(-1+n) + 31n + (\frac{48\sqrt{3} + 28\sqrt{2}}{21})(2+n) \\ &+ \frac{16}{5}\sqrt{6}(1+2n) + \frac{12}{11}\sqrt{30}(-1+4n). \end{aligned}$$

Proof. By using edge partition given in Table 3, we get the result. From (5) it follows that

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{deg(u) + deg(v) - 2}{deg(u) \cdot deg(v)}} = \sum_{j=1}^{8} \sum_{uv \in E_j(G)} \sqrt{\frac{deg(u) + deg(v) - 2}{deg(u) \cdot deg(v)}}.$$

Then, we have

$$\begin{aligned} ABC(G) &= \frac{\sqrt{15}}{6}|E_1(B_{36}(n))| + \frac{\sqrt{14}}{6}|E_2(B_{36}(n))| + \frac{\sqrt{6}}{4}|E_3(B_{36}(n))| \\ &+ \frac{\sqrt{35}}{10}|E_4(B_{36}(n))| + \frac{\sqrt{3}}{3}|E_5(B_{36}(n))| + 2\frac{\sqrt{2}}{5}|E_6(B_{36}(n))| \\ &+ \frac{\sqrt{30}}{10}|E_7(B_{36}(n))| + \frac{\sqrt{10}}{6}|E_8(B_{36}(n))|. \end{aligned}$$

By doing some calculation, we get

$$ABC(G) = \frac{1}{60}(24\sqrt{35}(-1+n) + 144\sqrt{2}n + (20\sqrt{14} + 40\sqrt{15})(2+n) + (160\sqrt{3} + 30\sqrt{6})(1+2n) + 36\sqrt{30}(-1+4n) + 30\sqrt{10}(-3+7n)).$$

From (6) we get

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{deg(u)deg(v)}}{(deg(u)+deg(v))} = \sum_{j=1}^{8} \sum_{uv \in E_j(G)} \frac{2\sqrt{deg(u)deg(v)}}{(deg(u)+deg(v))}.$$

By doing some calculation, we get

$$GA(G) = 4\frac{\sqrt{3}}{7}|E_1(B_{36}(n))| + 2\frac{2}{3}|E_2(B_{36}(n))| + |E_3(B_{36}(n))| + 4\frac{\sqrt{5}}{9}|E_4(B_{36}(n))| + 2\frac{\sqrt{6}}{5}|E_5(B_{36}(n))| + |E_6(B_{36}(n))| + 2\frac{\sqrt{30}}{11}|E_7(B_{36}(n))| + |E_8(B_{36}(n))|.$$

We have

$$GA(G) = -7 + \frac{16}{9}\sqrt{5}(-1+n) + 31n + (\frac{48\sqrt{3}+28\sqrt{2}}{21})(2+n) + \frac{16}{5}\sqrt{6}(1+2n) + \frac{12}{11}\sqrt{30}(-1+4n).$$

□

Now, we compute ABC_4 and GA_5 indices of borophene chain $B_{36}(n)$. Let us consider an edge partition based on degree sum of neighbors of end vertices. Then the edge set $E(B_{36}(n))$ can be divided into twenty four edge partitions $E_j(B_{36}(n)), 9 \leq j \leq 28$, where the edge partition $E_9(B_{36}(n))$ contains $4n+8$ edges uv with $S_u = 14$ and $S_v = 19$, the edge partition $E_{10}(B_{36}(n))$ contains $2n+4$ edges uv with $S_u = 14$ and $S_v = 28$, the edge partition $E_{11}(B_{36}(n))$ contains 6 edges uv with $S_u = S_v = 19$, the edge partition $E_{12}(B_{36}(n))$ contains $4n-4$ edges uv with $S_u = 19$ and $S_v = 20$, the edge partition $E_{13}(B_{36}(n))$ contains $4n+8$ edges uv with $S_u = 19$ and $S_v = 28$, the edge partition $E_{14}(B_{36}(n))$ contains $4n+8$ edges uv with $S_u = 19$ and $S_v = 30$, the edge partition $E_{15}(B_{36}(n))$ contains $4n-4$ edges uv with $S_u = 20$ and $S_v = 26$, $E_{16}(B_{36}(n))$ contains $4n-4$ edges uv with $S_u = 20$ and $S_v = 30$, $E_{17}(B_{36}(n))$ contains $4n-4$ edges uv with $S_u = 20$ and $S_v = 31$, $E_{18}(B_{36}(n))$ contains $4n-4$ edges uv with $S_u = 26$ and $S_v = 31$, $E_{19}(B_{36}(n))$ contains $2n-2$ edges uv with $S_u = 26$ and $S_v = 35$, $E_{20}(B_{36}(n))$ contains $8n+4$ edges uv with $S_u = S_v = 28$, $E_{21}(B_{36}(n))$ contains $12n+12$ edges uv with $S_u = 28$ and $S_v = 30$, $E_{22}(B_{36}(n))$ contains $4n-4$ edges uv with $S_u = 28$ and $S_v = 31$, $E_{23}(B_{36}(n))$ contains $4n-4$ edges uv with $S_u = 28$ and $S_v = 34$, $E_{24}(B_{36}(n))$ contains $4n-4$ edges uv with $S_u = 30$ and $S_v = 31$, $E_{25}(B_{36}(n))$ contains $4n-4$ edges uv with $S_u = 31$ and $S_v = 34$, $E_{26}(B_{36}(n))$ contains $4n-4$ edges uv with $S_u = 31$ and $S_v = 35$, $E_{27}(B_{36}(n))$ contains $4n-4$ edges uv with $S_u = 34$ and $S_v = 35$ and $E_{28}(B_{36}(n))$ contains $n-1$ edges uv with $S_u = S_v = 35$.

Theorem 2.8. *Let $G \cong B_{36}(n)$ be the borophene chain, for $n \geq 2$, then*

$$\begin{aligned}ABC_4(G) &= \frac{36}{19} + (6\sqrt{\frac{14}{527}} + 2\sqrt{\frac{134}{595}} + 2\sqrt{\frac{30}{119}} + 2\sqrt{\frac{118}{465}} + \sqrt{\frac{118}{455}} + 2\sqrt{\frac{57}{217}} \\ &+ 2\sqrt{\frac{110}{403}} + 2\sqrt{\frac{22}{65}} + 2\sqrt{\frac{37}{95}} + \frac{4}{3}\sqrt{2} + \frac{2}{35}\sqrt{17} + \frac{14}{\sqrt{155}} + \frac{32}{\sqrt{1085}}) \\ &+ 4\sqrt{\frac{3}{5}}(1+n) + (6\sqrt{\frac{5}{133}} + 2\sqrt{\frac{94}{285}} + 2\sqrt{\frac{62}{133}} + \frac{2}{7}\sqrt{5})(2+n) + \frac{3}{7}\sqrt{6}(1+2n), \\ GA_5(G) &= 9 + (\frac{8}{5}\sqrt{6} + \frac{16}{39}\sqrt{95} + \frac{8}{23}\sqrt{130} + \frac{16}{51}\sqrt{155} + \frac{16}{59}\sqrt{217} + \frac{8}{31}\sqrt{238} + \frac{8}{57}\sqrt{806} \\ &+ \frac{4}{61}\sqrt{910} + \frac{8}{61}\sqrt{930} + \frac{8}{65}\sqrt{1054} + \frac{4}{33}\sqrt{1085} + \frac{8}{69}\sqrt{1190})(-1+n) + 9n \\ &+ \frac{24}{29}\sqrt{210}(1+n) + (\frac{4}{3}\sqrt{2} + \frac{16}{47}\sqrt{133} + \frac{8}{33}\sqrt{266} + \frac{16}{49}\sqrt{570})(2+n).\end{aligned}$$

Proof. By using edge partition given in Table 4, we get the result. From (7) it follows that

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}} = \sum_{j=9}^{28} \sum_{uv \in E_j(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}.$$

Then, we have

$$\begin{aligned}ABC_4(G) &= \sqrt{\frac{31}{266}}|E_9(B_{36}(n))| + \frac{1}{7}\sqrt{5}|E_{10}(B_{36}(n))| + \frac{6}{19}|E_{11}(B_{36}(n))| \\ &+ \frac{3}{2}\sqrt{\frac{5}{133}}|E_{13}(B_{36}(n))| + \sqrt{\frac{47}{570}}|E_{14}(B_{36}(n))| + \sqrt{\frac{15}{130}}|E_{14}(B_{36}(n))| \\ &+ \frac{1}{3}\sqrt{2}|E_{16}(B_{36}(n))| + \frac{7}{2\sqrt{155}}|E_{17}(B_{36}(n))| + \sqrt{\frac{55}{806}}|E_{18}(B_{36}(n))| \\ &+ \sqrt{\frac{59}{910}}|E_{19}(B_{36}(n))| + \frac{3}{28}\sqrt{6}|E_{20}(B_{36}(n))| + \frac{\sqrt{15}}{15}|E_{21}(B_{36}(n))| \\ &+ \frac{1}{2}\sqrt{\frac{57}{217}}|E_{22}(B_{36}(n))| + \sqrt{\frac{15}{238}}|E_{23}(B_{36}(n))| + \sqrt{\frac{59}{930}}|E_{24}(B_{36}(n))| \\ &+ 3\sqrt{\frac{7}{1054}}|E_{25}(B_{36}(n))| + \frac{8}{\sqrt{1085}}|E_{26}(B_{36}(n))| + \sqrt{\frac{67}{1190}}|E_{27}(B_{36}(n))| \\ &+ \frac{2}{35}\sqrt{17}|E_{28}(B_{36}(n))| + \frac{1}{2}\sqrt{\frac{37}{95}}|E_{12}(B_{36}(n))|.\end{aligned}$$

Thus, we have

$$\begin{aligned}ABC_4(G) &= \frac{36}{19} + (6\sqrt{\frac{14}{527}} + 2\sqrt{\frac{134}{595}} + 2\sqrt{\frac{30}{119}} + 2\sqrt{\frac{118}{465}} + \sqrt{\frac{118}{455}} + 2\sqrt{\frac{57}{217}} + 2\sqrt{\frac{110}{403}} \\ &+ 2\sqrt{\frac{22}{65}} + 2\sqrt{\frac{37}{95}} + \frac{4}{3}\sqrt{2} + \frac{2}{35}\sqrt{17} + \frac{14}{\sqrt{155}} + \frac{32}{\sqrt{1085}}) + 4\sqrt{\frac{3}{5}}(1+n) \\ &+ (6\sqrt{\frac{5}{133}} + 2\sqrt{\frac{94}{285}} + 2\sqrt{\frac{62}{133}} + \frac{2}{7}\sqrt{5})(2+n) + \frac{3}{7}\sqrt{6}(1+2n),\end{aligned}$$

(S_u,S_v), $uv \in E(G)$	Number of edges	(S_u,S_v), $uv \in E(G)$	Number of edges
(14,19)	$4n+8$	(26,35)	$2n-2$
(14,28)	$2n+4$	(28,28)	$8n+4$
(19,19)	6	(28,30)	$12n+12$
(19,20)	$4n-4$	(28,31)	$4n-4$
(19,28)	$4n+8$	(28,34)	$4n-4$
(19,30)	$4n+8$	(30,31)	$4n-4$
(20,26)	$4n-4$	(31,34)	$4n-4$
(20,30)	$4n-4$	(31,35)	$4n-4$
(20,31)	$4n-4$	(34,35)	$4n-4$
(26,31)	$4n-4$	(35,35)	$n-1$

Table 4. Edge partition of borophene chain $B_{36}(n)$ based on degrees sum of end vertices of each edge.

and from (8) we get

$$GA_5(G) = \sum_{uv\in E(G)} \frac{2\sqrt{S_uS_v}}{(S_u+S_v)} = \sum_{j=9}^{28}\sum_{uv\in E_j(G)} \frac{2\sqrt{S_uS_v}}{(S_u+S_v)}.$$

Then, we have

$$\begin{aligned}
GA_5(G) &= \frac{2}{33}\sqrt{266}|E_9(B_{36}(n))| + \frac{2}{3}\sqrt{2}|E_{10}(B_{36}(n))| + |E_{11}(B_{36}(n))| \\
&+ \frac{4}{39}\sqrt{95}|E_{12}(B_{36}(n))| + \frac{4}{47}\sqrt{133}|E_{13}(B_{36}(n))| + \frac{4}{49}\sqrt{570}|E_{14}(B_{36}(n))| \\
&+ \frac{2}{23}\sqrt{130}|E_{15}(B_{36}(n))| + \frac{2}{5}\sqrt{6}|E_{16}(B_{36}(n))| + \frac{4}{51}\sqrt{155}|E_{17}(B_{36}(n))| \\
&+ \frac{2}{57}\sqrt{806}|E_{18}(B_{36}(n))| + \frac{2}{61}\sqrt{910}|E_{19}(B_{36}(n))| + |E_{20}(B_{36}(n))| \\
&+ \frac{2}{29}\sqrt{210}|E_{21}(B_{36}(n))| + \frac{4}{59}\sqrt{214}|E_{22}(B_{36}(n))| + \frac{2}{31}\sqrt{238}|E_{23}(B_{36}(n))| \\
&+ \frac{2}{61}\sqrt{930}|E_{24}(B_{36}(n))| + \frac{2}{65}\sqrt{1054}|E_{25}(B_{36}(n))| + \frac{1}{33}\sqrt{1085}|E_{26}(B_{36}(n))| \\
&+ \frac{2}{69}\sqrt{1190}|E_{27}(B_{36}(n))| + |E_{28}(B_{36}(n))| \\
&= 9 + (\frac{8}{5}\sqrt{6} + \frac{16}{39}\sqrt{95} + \frac{8}{23}\sqrt{130} + \frac{16}{51}\sqrt{155} + \frac{16}{59}\sqrt{217} + \frac{8}{31}\sqrt{238} + \frac{8}{57}\sqrt{806} \\
&+ \frac{4}{61}\sqrt{910} + \frac{8}{61}\sqrt{930} + \frac{8}{65}\sqrt{1054} + \frac{4}{33}\sqrt{1085} + \frac{8}{69}\sqrt{1190})(-1+n) + 9n \\
&+ \frac{24}{29}\sqrt{210}(1+n) + (\frac{4}{3}\sqrt{2} + \frac{16}{47}\sqrt{133} + \frac{8}{33}\sqrt{266} + \frac{16}{49}\sqrt{570})(2+n).
\end{aligned}$$

□

The melem (2, 5, 8-triamino-tri-s-triazine) $C_6N_7(NH_2)_3$ chain nanotube. The melem was obtained as a crystalline powder by thermal treatment of different less condensed $C-N-H$

compounds (e.g., melamine $C_3N_3(NH_2)_3$, dicyandiamide $H_4C_2N_4$, ammonium dicyanamide $NH_4[N(CN)_2]$, or cyanamide H_2CN_2, respectively) at temperatures up to $450°C$ in sealed glass ampules. The vertices and edges in melem chain are $18n+4$ and $21n+3$ respectively.

Now we compute Randić $R_\alpha(G)$ with $\alpha = \{1, -1, \frac{1}{2}, -\frac{1}{2}\}$, ABC, GA, ABC_4 and GA_5 indices for melem chain $MC(n)$ nanotube.

Theorem 2.9. *Consider the melem chain $MC(n)$ for $n \in \mathbb{N}$. Then*

$$R_\alpha(MC(n)) = \begin{cases} 135n+9, & \alpha = 1; \\ 3(6n+4\sqrt{6}n+\sqrt{3}(1+n)), & \alpha = \frac{1}{2}; \\ 1+\frac{11n}{3}, & \alpha = -1; \\ \sqrt{3}+(2+\sqrt{3}+2\sqrt{6})n, & \alpha = -\frac{1}{2}. \end{cases}$$

Proof. Let G be the melem chain. The melem chain $MC(n)$ has $3n+3$ vertices of degree 1, $6n$ vertices of degree 2, and $9n+1$ vertices of degree 3. The edge set of $MC(n)$ is divided into three partitions based on the degree of end vertices. The first edge partition $E_1(MC(n))$ contains $3n+3$ edges uv, where $deg(u) = 1$ and $deg(v) = 3$. The second edge partition $E_2(MC(n))$ contains $12n$ edges uv, where $deg(u) = 2$ and $deg(v) = 3$. The third edge partition $E_3(MC(n))$ contains $6n$ edges uv, where $deg(u) = deg(v) = 3$. Table 5 shows such an edge partition of $MC(n)$. Thus from (3) is follows that

$$R_\alpha(G) = \sum_{uv \in E(G)} (deg(u)deg(v))^\alpha.$$

Now we apply the formula of $R_\alpha(G)$ for $\alpha = 1$

$$R_1(G) = \sum_{j=1}^{3} \sum_{uv \in E_j(G)} deg(u)deg(v).$$

By using edge partition given in Table 5, we get

$$R_1(G) = 3|E_1(MC(n))| + 6|E_2(MC(n))| + 9|E_3(MC(n))| = 135n+9.$$

We apply the formula of $R_\alpha(G)$ for $\alpha = \frac{1}{2}$

$$R_{\frac{1}{2}}(G) = \sum_{j=1}^{3} \sum_{uv \in E_j(G)} \sqrt{deg(u) \cdot deg(v)}.$$

By using edge partition given in Table 5, we get

$$\begin{aligned} R_{\frac{1}{2}}(G) &= \sqrt{3}|E_1(MC(n))| + \sqrt{6}|E_2(MC(n))| + 3|E_3(MC(n))| \\ &= 3(6n+4\sqrt{6}n+\sqrt{3}(1+n)). \end{aligned}$$

(d_u,d_v), $uv \in E(G)$	Number of edges
(1,3)	$3n+3$
(2,3)	$12n$
(3,3)	$6n$

Table 5. Edge partition of melem chain $MC(n)$ based on degrees of end vertices of each edge.

We apply the formula of $R_\alpha(G)$ for $\alpha = -1$

$$\begin{aligned} R_{-1}(G) &= \sum_{j=1}^{3} \sum_{uv \in E_j(G)} \frac{1}{deg(u) \cdot deg(v)} \\ &= \frac{1}{3}|E_1(MC(n))| + \frac{1}{6}|E_2(MC(n))| + \frac{1}{9}|E_3(MC(n))| \\ &= 1 + \frac{11n}{3}. \end{aligned}$$

We apply the formula of $R_\alpha(G)$ for $\alpha = -\frac{1}{2}$

$$\begin{aligned} R_{-\frac{1}{2}}(G) &= \sum_{j=1}^{3} \sum_{uv \in E_j(G)} \frac{1}{\sqrt{deg(u) \cdot deg(v)}} \\ &= \frac{1}{\sqrt{3}}|E_1(MC(n))| + \frac{1}{\sqrt{6}}|E_2(MC(n))| + \frac{1}{3}|E_3(MC(n))| \\ &= \sqrt{3} + (2 + \sqrt{3} + 2\sqrt{6})n. \end{aligned}$$

□

In the following theorem, we compute first Zagreb index of melem chain $MC(n)$.

Theorem 2.10. *For melem chain $G \cong MC(n)$ for $n \in \mathbb{N}$. Then*

$$M_1(MC(n)) = 12(1 + 9n).$$

Proof. Let G be the borophene chain $B_{36}(n)$. By using edge partition from Table 5, the result follows. From (4) we have

$$\begin{aligned} M_1(MC(n)) &= \sum_{uv \in E(G)} (deg(u) + deg(v)) \\ &= \sum_{j=1}^{3} \sum_{uv \in E_j(G)} (deg(u) + deg(v)) \\ &= 4|E_1(MC(n))| + 5|E_2(MC(n))| + 6|E_3(MC(n))|. \end{aligned}$$

By doing some calculation, we get $M_1(MC(n)) = 12(1 + 9n)$. □

Now, we compute ABC and GA indices of melem chain $MC(n)$.

Theorem 2.11. *Let $G \cong MC(n)$ be the melem chain, for $n \in \mathbf{N}$, then*

$$ABC(G) = \sqrt{6} + (4 + 6\sqrt{2} + \sqrt{6})n,$$
$$GA(G) = 6n + \frac{24\sqrt{6}}{5}n + \frac{3\sqrt{3}}{2}(1+n).$$

Proof. By using edge partition given in Table 5, we get the result. From (5) it follows that

$$\begin{aligned} ABC(G) &= \sum_{uv \in E(G)} \sqrt{\frac{deg(u) + deg(v) - 2}{deg(u) \cdot deg(v)}} \\ &= \sum_{j=1}^{3} \sum_{uv \in E_j(G)} \sqrt{\frac{deg(u) + deg(v) - 2}{deg(u) \cdot deg(v)}} \\ &= \sqrt{\frac{2}{3}}|E_1(MC(n))| + \frac{1}{\sqrt{2}}|E_2(MC(n))| + \frac{2}{3}|E_3(MC(n))|. \end{aligned}$$

By doing some calculation, we get $ABC(G) = \sqrt{6} + (4 + 6\sqrt{2} + \sqrt{6})n$, from (6) we get

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{deg(u)deg(v)}}{(deg(u) + deg(v))} = \sum_{j=1}^{3} \sum_{uv \in E_j(G)} \frac{2\sqrt{deg(u)deg(v)}}{(deg(u) + deg(v))}.$$

By doing some calculation, we get

$$\begin{aligned} GA(G) &= \frac{\sqrt{3}}{2}|E_1(MC(n))| + \frac{2\sqrt{6}}{5}|E_2(MC(n))| + |E_3(MC(n))|, \\ &= 6n + \frac{24\sqrt{6}}{5}n + \frac{3\sqrt{3}}{2}(1+n). \end{aligned}$$

□

Now, we compute ABC_4 and GA_5 indices of melem chain $MC(n)$. Let us consider an edge partition based on degree sum of neighbors of end vertices. Then the edge set $E(MC(n))$ can be divided into six edge partitions $E_j(MC(n)), 4 \leq j \leq 9$, where the edge partition $E_4(MC(n))$ contains $2n+4$ edges uv with $S_u = 3$ and $S_v = 5$, the edge partition $E_5(MC(n))$ contains $n-1$ edges uv with $S_u = 3$ and $S_v = 7$, the edge partition $E_6(MC(n))$ contains $n+2$ edges uv with $S_u = 5$ and $S_v = 7$, the edge partition $E_7(MC(n))$ contains $12n$ edges uv with $S_u = 6$ and $S_v = 7$, the edge partition $E_8(MC(n))$ contains $2n-2$ edges uv with $S_u = S_v = 7$ and the edge partition $E_9(MC(n))$ contains $3n$ edges uv with $S_u = 7$ and $S_v = 9$.

Theorem 2.12. *Let $G \cong MC(n)$ be the melem chain, for $n \geq 2$, then*

$$\begin{aligned} ABC_4(G) &= (2\sqrt{\frac{2}{21}} + \frac{4\sqrt{3}}{7})(-1+n) + (\sqrt{2} + 2\sqrt{\frac{66}{7}})n + (\sqrt{\frac{2}{7}} + 2\sqrt{\frac{2}{5}})(2+n), \\ GA_5(G) &= -2 + \frac{1}{5}\sqrt{21}(-1+n) + (2 + \frac{9\sqrt{7}}{8} + \frac{24\sqrt{42}}{13})n \\ &\quad + (\frac{1}{2}\sqrt{15} + \frac{1}{6}\sqrt{35})(2+n). \end{aligned}$$

(S_u, S_v), $uv \in E(G)$	Number of edges
(3,5)	$2n+4$
(3,7)	$n-1$
(5,7)	$n+2$
(6,7)	$12n$
(7,7)	$2n-2$
(7,9)	$3n$

Table 6. Edge partition of Melem chain $MC(n)$ based on degrees sum of end vertices of each edge.

Proof. By using edge partition given in Table 6, we get the result. From (7) it follows that

$$\begin{aligned} ABC_4(G) &= \sum_{uv\in E(G)} \sqrt{\frac{S_u+S_v-2}{S_uS_v}} = \sum_{j=4}^{9}\sum_{uv\in E_j(G)} \sqrt{\frac{S_u+S_v-2}{S_uS_v}} \\ &= \sqrt{\frac{2}{5}}|E_4(MC(n))| + \frac{2\sqrt{2}}{\sqrt{21}}|E_5(MC(n))| + \sqrt{\frac{2}{7}}|E_6(MC(n))| \\ &+ \sqrt{\frac{11}{42}}|E_7(MC(n))| + \frac{2\sqrt{3}}{7}|E_8(MC(n))| + \frac{\sqrt{2}}{3}|E_9(MC(n))| \\ &= (2\sqrt{\frac{2}{21}} + \frac{4\sqrt{3}}{7})(-1+n) + (\sqrt{2}+2\sqrt{\frac{66}{7}})n + (\sqrt{\frac{2}{7}}+2\sqrt{\frac{2}{5}})(2+n), \end{aligned}$$

and from (8) we get

$$\begin{aligned} GA_5(G) &= \sum_{uv\in E(G)} \frac{2\sqrt{S_uS_v}}{(S_u+S_v)} = \sum_{j=4}^{9}\sum_{uv\in E_j(G)} \frac{2\sqrt{S_uS_v}}{(S_u+S_v)} \\ &= \frac{\sqrt{15}}{4}|E_4(MC(n))| + \frac{\sqrt{21}}{5}|E_5(MC(n))| + \frac{\sqrt{35}}{6}|E_6(MC(n))| \\ &+ \frac{2\sqrt{42}}{13}|E_7(MC(n))| + |E_8(MC(n))| + \frac{\sqrt{63}}{8}|E_9(MC(n))| \\ &= -2 + \frac{1}{5}\sqrt{21}(-1+n) + (2+\frac{9\sqrt{7}}{8} + \frac{24\sqrt{42}}{13})n + (\frac{1}{2}\sqrt{15}+\frac{1}{6}\sqrt{35})(2+n). \end{aligned}$$

□

3 Conclusion

In this paper, certain degree based topological indices, namely general Randić index, atomic-bond connectivity index (ABC), geometric-arithmetic index (GA) and first Zagreb index for boron triangular sheet $BTS(m,n)$, borophene chain of $B_{36}(n)$ and melem chain $MC(n)$ were studied for the first time and analytical closed formulas for these nanostructure were determined which will help the people working in chemical science to understand and explore the underlying topologies of these nanostructures.

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