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Computing Topological Indices of Two-Dimensional Lattice of Cu – BHS Nanocrystal Structure

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Abstract: In theoretical chemistry, distance, degree, and counting-related topological indices are introduced to study the properties of molecular topology; among these, degree-based topological indices are the most significant for their chemical properties. In this paper, we compute the general Randić index $R_\alpha(G)$ for different values of α, the first Zagreb index, the hyper Zagreb index, atom-bond connectivity (*ABC*) index, geometric arithmetic (*GA*) index, multiple Zagreb indices, the fourth *ABC* index and the fifth *GA* index for the two-dimensional lattice of *Cu – BHS* nanocrystal structure.

Keywords: Randić index; Zagreb type indices; atom-bond connectivity index; geometric arithmetic index; nanocrystal structure.

1. Introduction

All graphs considered in this paper are simple, connected, and undirected. Let $G = (V, E)$ be a graph with vertex set $V(G)$ and edge set $E(G)$. For an edge uv, we call u and v the end vertices of uv. For any vertex, u of G, $N_G(u)$ denotes the set of neighbors that u has in G. The set $N_G(u)$ is called the open neighborhood of u, and $N_G[u] = N_G(u) \cup \{u\}$ is called the closed neighborhood of u in G. The degree of a vertex u of G, denoted $\delta(u)$, is given by $\delta(u) = |N_G(u)|$.

Chemical systems may be depicted by chemical graphs using the atoms as the vertices of the graph and the molecular bonds as the edges. A special class of chemical graphs is molecular graphs that represent molecule's constitutions [1]. The topological index is a numerical parameter measured based on a chemical constitution's molecular graph. There are many distance or degree or counting related topological indices. Among these, degree-based topological indices are recognized as useful chemical research tools. One can refer to the articles [2–17] for a recent study on topological indices.

One of the oldest degree-based topological indices is the Randić index which was introduced by Milan Randić and defined [18] as follows:

$$R_{-\frac{1}{2}}(G) = \sum_{v_1v_2\in E(G)} \frac{1}{\sqrt{\delta(v_1)\times\delta(v_2)}}$$

The general Randić index $R_\alpha(G)$ is defined [19] as

$$R_\alpha(G) = \sum_{v_1v_2\in E(G)} (\delta(v_1)\times\delta(v_2))^\alpha; \alpha = 1, \frac{1}{2}, -1, \frac{-1}{2}$$

The first Zagreb index is a degree-based topological index that Gutman and Trinajstic introduced and defined [20] as follows:

$$M_1(G) = \sum_{v_1v_2 \in E(G)} [\delta(v_1) + \delta(v_2)]$$

The hyper Zagreb index is defined [21] as

$$HM(G) = \sum_{v_1v_2 \in E(G)} [\delta(v_1) + \delta(v_2)]^2$$

An important degree-based topological index is the *ABC* index introduced by Estrada *et al*. in [22] and defined as follows:

$$ABC(G) = \sum_{v_1v_2 \in E(G)} \sqrt{\frac{\delta(v_1) + \delta(v_2) - 2}{\delta(v_1) \times \delta(v_2)}}$$

Vukičevič and Furtula [23] defined the *GA* index as

$$GA(G) = \sum_{v_1v_2 \in E(G)} \frac{2\sqrt{\delta(v_1) \times \delta(v_2)}}{\delta(v_1) + \delta(v_2)}$$

Ghorbani and Azimi defined [24] the first and second multiple Zagreb indices as

$$PM_1(G) = \prod_{v_1v_2 \in E(G)} [\delta(v_1) + \delta(v_2)]$$

$$PM_2(G) = \prod_{v_1v_2 \in E(G)} [\delta(v_1) \times \delta(v_2)]$$

Ghorbani *et al.* [25] introduced the fourth version of the *ABC* index and defined it as follows:

$$ABC_4(G) = \sum_{v_1v_2 \in E(G)} \sqrt{\frac{S_{v_1} + S_{v_2} - 2}{S_{v_1} \times S_{v_2}}}$$

where $S_{v_1} = \sum_{v_2 \in N_G(v_1)} \delta(v_2)$.

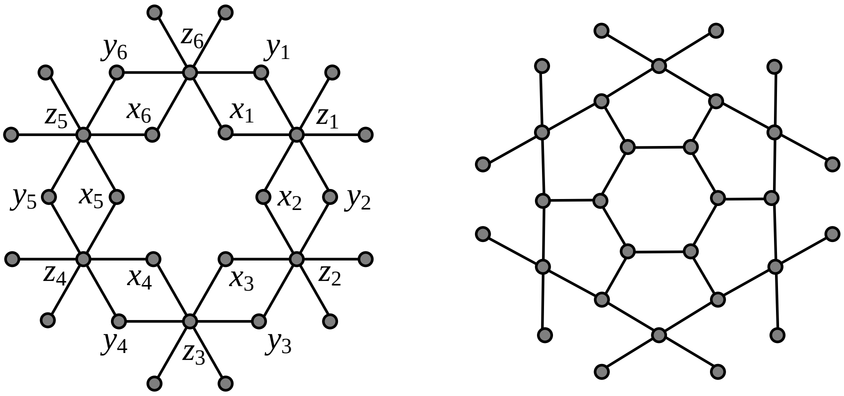
Graovac *et al.* [26] proposed the fifth version of the *GA* index and defined it as

$$GA_5(G) = \sum_{v_1v_2 \in E(G)} \frac{2\sqrt{S_{v_1} \times S_{v_2}}}{(S_{v_1} + S_{v_2})}$$

In this paper, we compute formulas of $R_\alpha(G)$ for different values of α, $M_1(G)$, $HM(G)$, $ABC(G)$, $GA(G)$, $PM_1(G)$, $PM_2(G)$, $ABC_4(G)$ and $GA_5(G)$ for the two-dimensional lattice of Cu – BHS nanocrystal structures.

2. The Two Dimensional Lattice of Cu – BHS

In recent times designing new architectures from the perspective of chem-informatics has gained importance among researchers. In particular, two-dimensional nanocrystals have received great research interest. Krishnan *et al*. [27] have designed an architecture based on the bismuth molecule. Recently Imran *et al*. [28] computed certain topological indices for the bismuth tri-iodide chain and sheet graph. In this section, we compute certain topological indices of the graph of the two-dimensional lattice of Cu – BHS nanocrystal structures.



(*i*) (*ii*)

Figure 1. (**i**) One unit of BiI_3 (**ii**) One unit of Cu – BHS.

Two-dimensional nanocrystals are crystalline materials that have one dimension (usually their thickness) on the nanometre scale. The nanocrystals of copper bis(diselenolene) (Cu – BHS) are synthesized via a simple homogeneous reaction between cupric ions and benzenehexaselenol (H_6BHS). It is made up of carbon, copper, and selenium ions [29].

The graph of a single unit of Cu – BHS can be obtained from the graph of a single unit of bismuth tri-iodide BiI_3 by adding the edges $(x_i, x_{i+1}), (x_i, y_i)$, $1 \leq i \leq 6$, and then deleting the edges $(x_i, z_i), (x_{i+1}, z_i)$, $1 \leq i \leq 6$. It is assumed that $x_6 = x_1$. Figure 1 (*i*) depicts the graph of one unit of BiI_3, and (*ii*) depicts the graph of one unit of Cu – BHS.

The unit cells of Cu – BHS can be arranged either linearly or in a sheet form. A linear arrangement with *m* unit cells is called an *m*-Cu – BHS chain (Figure 2); *mn* unit cells arranged into *m* rows and *n* columns are called an *m* × *n*-Cu – BHS sheet (Figure 3).

Theorem 2.1 Let *G* be *m* × *n*-Cu – BHS nanosheet. Then the number of vertices and edges of *G* are $15mn + 8m + 8n - 1$ and $24mn + 8m + 8n - 4$.

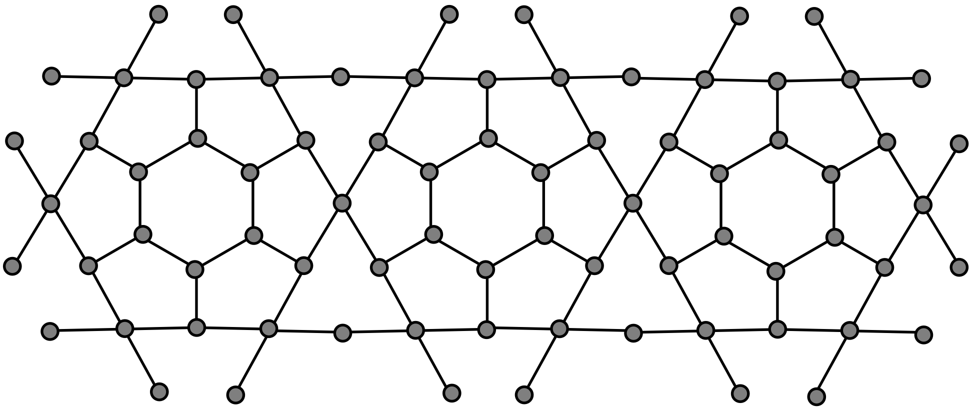


Figure 2. A 3-Cu – BHS chain.

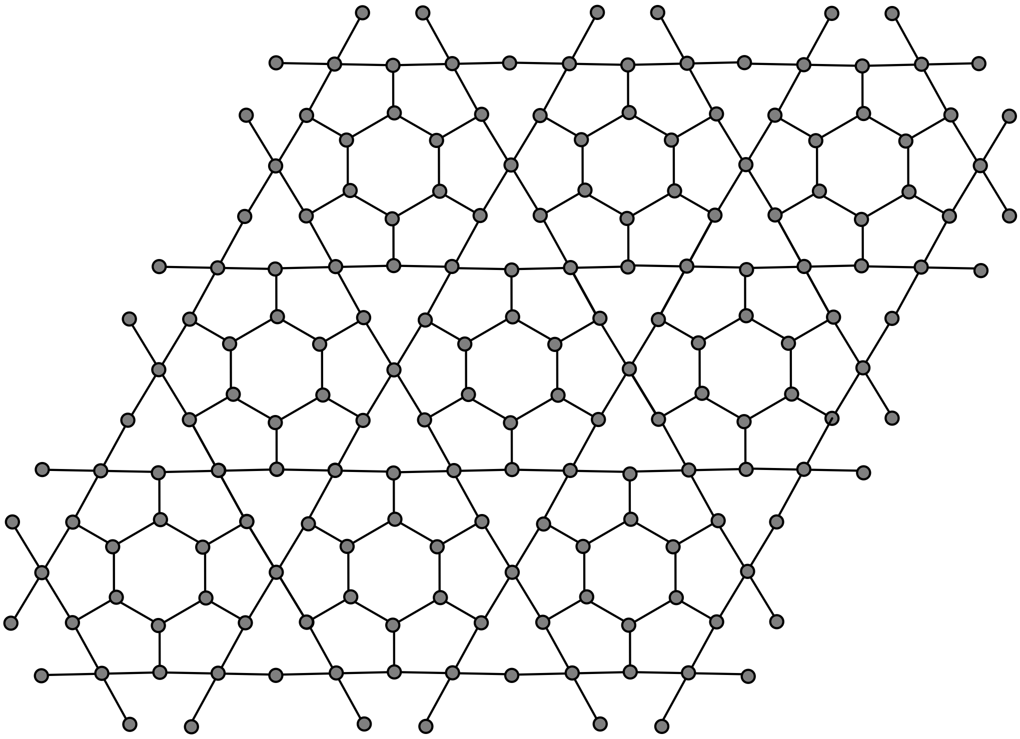


Figure 3. A 3 × 3-Cu – BHS sheet.

It is clear that G has $4m + 4n + 4$ vertices of degree 1, $2m + 2n - 4$ vertices of degree 2, $12mn$ vertices of degree 3, and $3mn + 2m + 2n - 1$ vertices of degree 4.

Table 1. Number of edges in each set of the partition.

$(\delta_{v_1}, \delta_{v_2})$ **where** $v_1v_2 \in E(G)$	**Number of edges**
(1, 4)	$4m + 4n + 4$
(2, 4)	$4m + 4n - 8$
(3, 3)	$12mn$
(3, 4)	$12mn$

We now compute the general Randić index $R_\alpha(G)$ for different values of α.

Theorem 2.2 Let G be $m \times n$- Cu – BHS. Then

$$R_\alpha(G) = \begin{cases} 252mn + 48m + 48n - 48, & \alpha = 1; \\ 12(3+\sqrt{12})mn + (1+\sqrt{2})m + (1+\sqrt{2})n + 8(1-\sqrt{8}), & \alpha = \frac{1}{2}; \\ \frac{7}{3}mn + \frac{3}{2}m + \frac{3}{2}n, & \alpha = -1; \\ (4+\sqrt{12})mn + (2+\sqrt{2})m + (2+\sqrt{2})n + 2(1-\sqrt{2}), & \alpha = \frac{-1}{2}. \end{cases}$$

Proof.

Consider graph G. Define a set $E_{ij}(G) \subset E(G)$ as $E_{ij}(G) = \{v_1v_2 \in E(G): \delta(v_1) = i, \delta(v_2) = j\}$. Then it is clear that $E(G) = E_{14}(G) \cup E_{24}(G) \cup E_{33}(G) \cup E_{34}(G)$ where

$$E_{14}(G) = \{v_1v_2 \in E(G): \delta(v_1) = 1, \delta(v_2) = 4\}$$
$$E_{24}(G) = \{v_1v_2 \in E(G): \delta(v_1) = 2, \delta(v_2) = 4\}$$
$$E_{33}(G) = \{v_1v_2 \in E(G): \delta(v_1) = 3, \delta(v_2) = 3\}$$
$$E_{34}(G) = \{v_1v_2 \in E(G): \delta(v_1) = 3, \delta(v_2) = 4\}$$

By definition of the Randić index $R_\alpha(G)$ for $\alpha = 1, \frac{1}{2}, -1, \frac{-1}{2}$ and using the values from Table 1, we get

$$
\begin{aligned}
R_1(G) &= \sum_{v_1v_2\in E(G)} [\delta(v_1)\times\delta(v_2)] \\
&= \sum_{v_1v_2\in E_{14}(G)} [\delta(v_1)\times\delta(v_2)] + \sum_{v_1v_2\in E_{24}(G)} [\delta(v_1)\times\delta(v_2)] + \\
&\quad + \sum_{v_1v_2\in E_{33}(G)} [\delta(v_1)\times\delta(v_2)] + \sum_{v_1v_2\in E_{34}(G)} [\delta(v_1)\times\delta(v_2)] \\
&= 4|E_{14}(G)| + 8|E_{24}(G)| + 9|E_{33}(G)| + 12|E_{34}(G)| \\
&= 4(4m+4n+4) + 8(4m+4n-8) + 9(12mn) + 12(12mn) \\
&= 252mn + 48m + 48n - 48.
\end{aligned}
$$

$$
\begin{aligned}
R_{\frac{1}{2}}(G) &= \sum_{v_1v_2\in E(G)} \sqrt{\delta(v_1)\times\delta(v_2)} \\
&= \sum_{v_1v_2\in E_{14}(G)} \sqrt{\delta(v_1)\times\delta(v_2)} + \sum_{v_1v_2\in E_{24}(G)} \sqrt{\delta(v_1)\times\delta(v_2)} + \\
&\quad + \sum_{v_1v_2\in E_{33}(G)} \sqrt{\delta(v_1)\times\delta(v_2)} + \sum_{v_1v_2\in E_{34}(G)} \sqrt{\delta(v_1)\times\delta(v_2)} \\
&= \sqrt{4}|E_{14}(G)| + \sqrt{8}|E_{24}(G)| + \sqrt{9}|E_{33}(G)| + \sqrt{12}|E_{34}(G)| \\
&= 2(4m+4n+4) + \sqrt{8}(4m+4n-8) + 3(12mn) + \sqrt{12}(12mn) \\
&= 12\left(3+\sqrt{12}\right)mn + \left(1+\sqrt{2}\right)m + \left(1+\sqrt{2}\right)n + 8\left(1-\sqrt{8}\right).
\end{aligned}
$$

$$
\begin{aligned}
R_{-1}(G) &= \sum_{v_1v_2\in E(G)} \frac{1}{\delta(v_1)\times\delta(v_2)} \\
&= \sum_{v_1v_2\in E_{14}(G)} \frac{1}{\delta(v_1)\times\delta(v_2)} + \sum_{v_1v_2\in E_{24}(G)} \frac{1}{\delta(v_1)\times\delta(v_2)} + \sum_{v_1v_2\in E_{33}(G)} \frac{1}{\delta(v_1)\times\delta(v_2)} \\
&\quad + \sum_{v_1v_2\in E_{34}(G)} \frac{1}{\delta(v_1)\times\delta(v_2)} \\
&= \frac{1}{4}|E_{14}(G)| + \frac{1}{8}|E_{24}(G)| + \frac{1}{9}|E_{33}(G)| + \frac{1}{12}|E_{34}(G)| \\
&= \frac{1}{4}(4m+4n+4) + \frac{1}{8}(4m+4n-8) + \frac{1}{9}(12mn) + \frac{1}{12}(12mn) \\
&= \frac{7}{3}mn + \frac{3}{2}m + \frac{3}{2}n.
\end{aligned}
$$

$$
\begin{aligned}
R_{-\frac{1}{2}}(G) &= \sum_{v_1v_2\in E(G)} \frac{1}{\sqrt{\delta(v_1)\times\delta(v_2)}} \\
&= \sum_{v_1v_2\in E_{14}(G)} \frac{1}{\sqrt{\delta(v_1)\times\delta(v_2)}} + \sum_{v_1v_2\in E_{24}(G)} \frac{1}{\sqrt{\delta(v_1)\times\delta(v_2)}} \\
&\quad + + \sum_{v_1v_2\in E_{33}(G)} \frac{1}{\sqrt{\delta(v_1)\times\delta(v_2)}} + \sum_{v_1v_2\in E_{34}(G)} \frac{1}{\sqrt{\delta(v_1)\times\delta(v_2)}} \\
&= \frac{1}{\sqrt{4}}|E_{14}(G)| + \frac{1}{\sqrt{8}}|E_{24}(G)| + \frac{1}{\sqrt{9}}|E_{33}(G)| + \frac{1}{\sqrt{12}}|E_{34}(G)|
\end{aligned}
$$

$$= \frac{1}{2}(4m+4n+4) + \frac{1}{2\sqrt{2}}(4m+4n-8) + \frac{1}{3}(12mn) + \frac{1}{\sqrt{12}}(12mn)$$
$$= (4+\sqrt{12})mn + (2+\sqrt{2})m + (2+\sqrt{2})n + 2(1-\sqrt{2}).$$

Theorem 2.3 Let *G* be *m* × *n*- Cu – BHS. Then
1. $M_1(G) = 156mn + 44m + 44n - 28.$
2. $HM(G) = 1020mn + 244m + 244n - 188.$

Proof. From the definition of the first Zagreb index, hyper Zagreb index, and by using Table 1, we obtain

$$M_1(G) = \sum_{v_1v_2 \in E(G)} [\delta(v_1) + \delta(v_2)]$$
$$= \sum_{v_1v_2 \in E_{14}(G)} [\delta(v_1) + \delta(v_2)] + \sum_{v_1v_2 \in E_{24}(G)} [\delta(v_1) + \delta(v_2)]$$
$$+ \sum_{v_1v_2 \in E_{33}(G)} [\delta(v_1) + \delta(v_2)] + \sum_{v_1v_2 \in E_{34}(G)} [\delta(v_1) + \delta(v_2)]$$
$$= 5|E_{14}(G)| + 6|E_{24}(G)| + 6|E_{33}(G)| + 7|E_{34}(G)|$$
$$= 5(4m+4n+4) + 6(4m+4n-8) + 6(12mn) + 7(12mn)$$
$$= 156mn + 44m + 44n - 28.$$

$$HM(G) = \sum_{v_1v_2 \in E(G)} [\delta(v_1) + \delta(v_2)]^2$$
$$= \sum_{v_1v_2 \in E_{14}(G)} [\delta(v_1) + \delta(v_2)]^2 + \sum_{v_1v_2 \in E_{24}(G)} [\delta(v_1) + \delta(v_2)]^2 +$$
$$\sum_{v_1v_2 \in E_{33}(G)} [\delta(v_1) + \delta(v_2)]^2 + \sum_{v_1v_2 \in E_{34}(G)} [\delta(v_1) + \delta(v_2)]^2$$
$$= 5^2|E_{14}(G)| + 6^2|E_{24}(G)| + 6^2|E_{33}(G)| + 7^2|E_{34}(G)|$$
$$= 25(4m+4n+4) + 36(4m+4n-8) + 36(12mn) + 49(12mn)$$
$$= 1020mn + 244m + 244n - 188.$$

Theorem 2.4 Let *G* be *m* × *n*- Cu – BHS. Then
1. $ABC(G) = (8+2\sqrt{15})mn + 2(\sqrt{2}+\sqrt{3})m + 2(\sqrt{2}+\sqrt{3})n + 2\sqrt{3} - 4\sqrt{2}.$
2. $GA(G) = \left(\frac{84+48\sqrt{3}}{7}\right)mn + \left(\frac{48+20\sqrt{8}}{15}\right)m + \left(\frac{48+20\sqrt{8}}{15}\right)n + \left(\frac{48-40\sqrt{8}}{15}\right).$

Proof. By the definition of *ABC* and *GA* indices and using the values from Table 1, we get

$$ABC(G) = \sum_{v_1v_2 \in E(G)} \sqrt{\frac{\delta(v_1) + \delta(v_2) - 2}{\delta(v_1) \times \delta(v_2)}}$$

$$= \sum_{v_1v_2 \in E_{14}(G)} \sqrt{\frac{\delta(v_1)+\delta(v_2)-2}{\delta(v_1)\times\delta(v_2)}} + \sum_{v_1v_2 \in E_{24}(G)} \sqrt{\frac{\delta(v_1)+\delta(v_2)-2}{\delta(v_1)\times\delta(v_2)}}$$
$$+ \sum_{v_1v_2 \in E_{33}(G)} \sqrt{\frac{\delta(v_1)+\delta(v_2)-2}{\delta(v_1)\times\delta(v_2)}} + \sum_{v_1v_2 \in E_{34}(G)} \sqrt{\frac{\delta(v_1)+\delta(v_2)-2}{\delta(v_1)\times\delta(v_2)}}$$
$$= \sqrt{\frac{3}{4}}(|E_{14}(G)|) + \sqrt{\frac{4}{8}}(|E_{24}(G)|) + \sqrt{\frac{4}{9}}(|E_{33}(G)|) + \sqrt{\frac{5}{12}}(|E_{34}(G)|)$$
$$= \sqrt{\frac{3}{4}}(4m+4n+4) + \sqrt{\frac{4}{8}}(4m+4n-8) + \sqrt{\frac{4}{9}}(12mn) + \sqrt{\frac{5}{12}}(12mn)$$
$$= (8+2\sqrt{15})mn + 2(\sqrt{2}+\sqrt{3})m + 2(\sqrt{2}+\sqrt{3})n + 2\sqrt{3} - 4\sqrt{2}.$$

$$GA(G) = \sum_{v_1v_2 \in E(G)} \frac{2\sqrt{\delta(v_1)\times\delta(v_2)}}{\delta(v_1)+\delta(v_2)}$$
$$= \sum_{v_1v_2 \in E_{14}(G)} \frac{2\sqrt{\delta(v_1)\times\delta(v_2)}}{\delta(v_1)+\delta(v_2)} + \sum_{v_1v_2 \in E_{24}(G)} \frac{2\sqrt{\delta(v_1)\times\delta(v_2)}}{\delta(v_1)+\delta(v_2)} +$$
$$+ \sum_{v_1v_2 \in E_{33}(G)} \frac{2\sqrt{\delta(v_1)\times\delta(v_2)}}{\delta(v_1)+\delta(v_2)} + \sum_{v_1v_2 \in E_{34}(G)} \frac{2\sqrt{\delta(v_1)\times\delta(v_2)}}{\delta(v_1)+\delta(v_2)}$$
$$= \frac{2\sqrt{4}}{5}(|E_{14}(G)|) + \frac{2\sqrt{8}}{6}(|E_{24}(G)|) + \frac{2\sqrt{9}}{6}(|E_{33}(G)|) + \frac{2\sqrt{12}}{7}(|E_{34}(G)|)$$
$$= \frac{2\sqrt{4}}{5}(4m+4n+4) + \frac{2\sqrt{8}}{6}(4m+4n-8) + \frac{2\sqrt{9}}{6}(12mn) + \frac{2\sqrt{12}}{7}(12mn)$$
$$= \left(\frac{84+48\sqrt{3}}{7}\right)mn + \left(\frac{48+20\sqrt{8}}{15}\right)m + \left(\frac{48+20\sqrt{8}}{15}\right)n + \left(\frac{48-40\sqrt{8}}{15}\right).$$

Theorem 2.5 Let G be $m \times n$- Cu – BHS. Then
1. $PM_1(G) = 5^{(4m+4n+4)} \times 6^{(12mn+4m+4n-8)} \times 7^{(12mn)}$.
2. $PM_2(G) = 4^{(4m+4n+4)} \times 8^{(4m+4n-8)} \times 9^{(12mn)} \times 12^{(12mn)}$.

Proof. By definition of multiple Zagreb indices and using the values from Table 1, we compute

$$PM_1(G) = \prod_{v_1v_2 \in E(G)} [\delta(v_1)+\delta(v_2)]$$
$$= \prod_{v_1v_2 \in E_{14}(G)} [\delta(v_1)+\delta(v_2)] \times \prod_{v_1v_2 \in E_{24}(G)} [\delta(v_1)+\delta(v_2)]$$
$$\times \prod_{v_1v_2 \in E_{33}(G)} [\delta(v_1)+\delta(v_2)] \times \prod_{v_1v_2 \in E_{34}(G)} [\delta(v_1)+\delta(v_2)]$$
$$= 5^{|E_{14}(G)|} \times 6^{|E_{24}(G)|} \times 6^{|E_{33}(G)|} \times 7^{|E_{34}(G)|}$$
$$= 5^{(4m+4n+4)} \times 6^{(4m+4n-8)} \times 6^{(12mn)} \times 7^{(12mn)}$$
$$= 5^{(4m+4n+4)} \times 6^{(12mn+4m+4n-8)} \times 7^{(12mn)}.$$

$$\begin{aligned}PM_2(G) &= \prod_{v_1v_2\in E(G)}[\delta(v_1)\times\delta(v_2)]\\ &= \prod_{v_1v_2\in E_{14}(G)}[\delta(v_1)\times\delta(v_2)] \times \prod_{v_1v_2\in E_{24}(G)}[\delta(v_1)\times\delta(v_2)]\\ &\qquad\qquad \times \prod_{v_1v_2\in E_{33}(G)}[\delta(v_1)\times\delta(v_2)] \times \prod_{v_1v_2\in E_{34}(G)}[\delta(v_1)\times\delta(v_2)]\\ &= 4^{|E_{14}(G)|}\times 8^{|E_{24}(G)|}\times 9^{|E_{33}(G)|}\times 12^{|E_{34}(G)|}\\ &= 4^{(4m+4n+4)}\times 8^{(4m+4n-8)}\times 9^{(12mn)}\times 12^{(12mn)}.\end{aligned}$$

Table 2. Number of edges in each set of the partition.

(S_{v_1}, S_{v_2}) where $v_1v_2 \in E(G)$	Number of edges
(4, 8)	12
(4, 9)	$4m + 4n - 8$
(8, 9)	$4m + 4n - 8$
(8, 11)	12
(9, 9)	$6mn$
(9, 11)	$6mn + 8m + 8n - 16$
(11, 12)	$12mn - 8m - 8n + 4$

There are seven types of edges based on the degree sum of end vertices of each edge of G. We define a set $E_{kl}(G) \subset E(G)$ as $E_{k,l}(G) = \{v_1v_2 \in E(G): S_{v_1} = k, S_{v_2} = l\}$. Clearly, $E(G) = E_{4,8}(G) \cup E_{4,9}(G) \cup E_{8,9}(G) \cup E_{8,11}(G) \cup E_{9,9}(G) \cup E_{9,11}(G) \cup E_{11,12}(G)$ where

$$E_{4,8}(G) = \{v_1v_2 \in E(G): S_{v_1} = 4, S_{v_2} = 8\}$$
$$E_{4,9}(G) = \{v_1v_2 \in E(G): S_{v_1} = 4, S_{v_2} = 9\}$$
$$E_{8,9}(G) = \{v_1v_2 \in E(G): S_{v_1} = 8, S_{v_2} = 9\}$$
$$E_{8,11}(G) = \{v_1v_2 \in E(G): S_{v_1} = 8, S_{v_2} = 11\}$$
$$E_{9,9}(G) = \{v_1v_2 \in E(G): S_{v_1} = 9, S_{v_2} = 9\}$$
$$E_{9,11}(G) = \{v_1v_2 \in E(G): S_{v_1} = 9, S_{v_2} = 11\}$$
$$E_{11,12}(G) = \{v_1v_2 \in E(G): S_{v_1} = 11, S_{v_2} = 12\}.$$

We use this partition of edges to calculate ABC_4 and GA_5 indices in the following theorem.

Theorem 2.6 Let *G* be *m* × *n*- Cu – BHS. Then

$$\begin{aligned}1.\ ABC_4(G) &= \left(6\sqrt{\frac{16}{81}} + 6\sqrt{\frac{18}{99}} + 12\sqrt{\frac{21}{132}}\right)mn + \left(4\sqrt{\frac{11}{36}} + 4\sqrt{\frac{15}{72}} + 8\sqrt{\frac{18}{99}} - 8\sqrt{\frac{21}{132}}\right)m\\ &+ \left(4\sqrt{\frac{11}{36}} + 4\sqrt{\frac{15}{72}} + 8\sqrt{\frac{18}{99}} - 8\sqrt{\frac{21}{132}}\right)n\\ &+ \left(12\sqrt{\frac{10}{32}} - 8\sqrt{\frac{11}{36}} - 8\sqrt{\frac{15}{72}} + 12\sqrt{\frac{17}{88}} - 16\sqrt{\frac{18}{99}} + 4\sqrt{\frac{21}{132}}\right).\end{aligned}$$

$$2.\, GA_5(G) = \left(\frac{2\sqrt{81}}{3} + \frac{3\sqrt{99}}{5} + \frac{24\sqrt{132}}{23}\right)mn + \left(\frac{8\sqrt{36}}{13} + \frac{8\sqrt{72}}{17} + \frac{4\sqrt{99}}{5} - \frac{16\sqrt{132}}{23}\right)m + \left(\frac{8\sqrt{36}}{13} + \frac{8\sqrt{72}}{17} + \frac{4\sqrt{99}}{5} - \frac{16\sqrt{132}}{23}\right)n + \left(2\sqrt{32} - \frac{16\sqrt{36}}{13} - \frac{16\sqrt{72}}{17} + \frac{24\sqrt{88}}{19} - \frac{8\sqrt{132}}{5}\right).$$

Proof. By applying the formula of ABC_4 and GA_5 indices, and by using the values from Table 2, we get

$$ABC_4(G) = \sum_{v_1v_2 \in E} \sqrt{\frac{S_{v_1} + S_{v_2} - 2}{S_{v_1} \times S_{v_2}}}$$

$$= |E_{4,8}|\sqrt{\frac{4+8-2}{4\times 8}} + |E_{4,9}|\sqrt{\frac{4+9-2}{4\times 9}} + |E_{8,9}|\sqrt{\frac{8+9-2}{8\times 9}} + |E_{8,11}|\sqrt{\frac{8+11-2}{8\times 11}} + |E_{9,9}|\sqrt{\frac{9+9-2}{9\times 9}} + |E_{9,11}|\sqrt{\frac{9+11-2}{9\times 11}} + |E_{11,12}|\sqrt{\frac{11+12-2}{11\times 12}}$$

$$= 12\sqrt{\frac{4+8-2}{4\times 8}} + (4m+4n-8)\sqrt{\frac{4+9-2}{4\times 9}} + (4m+4n-8)\sqrt{\frac{8+9-2}{8\times 9}} + 12\sqrt{\frac{8+11-2}{8\times 11}} + 6mn\sqrt{\frac{9+9-2}{9\times 9}} + (6mn+8m+8n-16)\sqrt{\frac{9+11-2}{9\times 11}} + (12mn-8m-8n+4)\sqrt{\frac{11+12-2}{11\times 12}}$$

$$= 12\sqrt{\frac{10}{32}} + (4m+4n-8)\sqrt{\frac{11}{36}} + (4m+4n-8)\sqrt{\frac{15}{72}} + 12\sqrt{\frac{17}{88}} + 6mn\sqrt{\frac{16}{81}} + (6mn+8m+8n-16)\sqrt{\frac{18}{99}} + (12mn-8m-8n+4)\sqrt{\frac{21}{132}}$$

$$= \left(6\sqrt{\frac{16}{81}} + 6\sqrt{\frac{18}{99}} + 12\sqrt{\frac{21}{132}}\right)mn + \left(4\sqrt{\frac{11}{36}} + 4\sqrt{\frac{15}{72}} + 8\sqrt{\frac{18}{99}} - 8\sqrt{\frac{21}{132}}\right)m + \left(4\sqrt{\frac{11}{36}} + 4\sqrt{\frac{15}{72}} + 8\sqrt{\frac{18}{99}} - 8\sqrt{\frac{21}{132}}\right)n + \left(12\sqrt{\frac{10}{32}} - 8\sqrt{\frac{11}{36}} - 8\sqrt{\frac{15}{72}} + 12\sqrt{\frac{17}{88}} - 16\sqrt{\frac{18}{99}} + 4\sqrt{\frac{21}{132}}\right).$$

$$GA_5(G) = \sum_{v_1v_2 \in E} \frac{2\sqrt{S_{v_1}S_{v_2}}}{(S_{v_1} + S_{v_2})}$$

$$= |E_{4,8}|\frac{2\sqrt{4\times 8}}{(4+8)} + |E_{4,9}|\frac{2\sqrt{4\times 9}}{(4+9)} + |E_{8,9}|\frac{2\sqrt{8\times 9}}{(8+9)} + |E_{8,11}|\frac{2\sqrt{8\times 11}}{(8+11)} + |E_{9,9}|\frac{2\sqrt{9\times 9}}{(9+9)} + |E_{9,11}|\frac{2\sqrt{9\times 11}}{(9+11)} + |E_{11,12}|\frac{2\sqrt{11\times 12}}{(11+12)}$$

$$= 12\left(\frac{2\sqrt{4\times 8}}{4+8}\right) + (4m+4n-8)\left(\frac{2\sqrt{4\times 9}}{4+9}\right) + (4m+4n-8)\left(\frac{2\sqrt{8\times 9}}{8+9}\right) + 12\left(\frac{2\sqrt{8\times 11}}{8+11}\right) + 6mn\left(\frac{2\sqrt{9\times 9}}{9+9}\right) + (6mn+8m+8n-16)\left(\frac{2\sqrt{9\times 11}}{9+11}\right) + (12mn-8m-8n+4)\left(\frac{2\sqrt{11\times 12}}{11+12}\right)$$

$$= 12\left(\frac{2\sqrt{32}}{12}\right) + (4m+4n-8)\left(\frac{2\sqrt{36}}{13}\right) + (4m+4n-8)\left(\frac{2\sqrt{72}}{17}\right) + 12\left(\frac{2\sqrt{88}}{19}\right) + 6mn\left(\frac{2\sqrt{81}}{18}\right) + (6mn+8m+8n-16)\left(\frac{2\sqrt{99}}{20}\right) + (12mn-8m-8n+4)\left(\frac{2\sqrt{132}}{23}\right)$$

$$= \left(\frac{2\sqrt{81}}{3} + \frac{3\sqrt{99}}{5} + \frac{24\sqrt{132}}{23}\right)mn + \left(\frac{8\sqrt{36}}{13} + \frac{8\sqrt{72}}{17} + \frac{4\sqrt{99}}{5} - \frac{16\sqrt{132}}{23}\right)m + \left(\frac{8\sqrt{36}}{13} + \frac{8\sqrt{72}}{17} + \frac{4\sqrt{99}}{5} - \frac{16\sqrt{132}}{23}\right)n + \left(2\sqrt{32} - \frac{16\sqrt{36}}{13} - \frac{16\sqrt{72}}{17} + \frac{24\sqrt{88}}{19} - \frac{8\sqrt{132}}{5}\right).$$

3. Conclusions

In the present work, certain degree-based topological indices are computed for the graph of the two-dimensional lattice of the Cu – BHS nanocrystal structure. In addition, the distance-based topological indices for the graph of the two-dimensional lattice of the Cu – BHS nanocrystal structure are under investigation.

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Conflicts of Interest

The authors declare that there is no conflict of interest regarding the publication of this article.

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