Research Article

The Atom-Bond Connectivity Index of Catacondensed Polyomino Graphs

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Let $G = (V,E)$ be a graph. The atom-bond connectivity (ABC) index is defined as the sum of weights $\left(\frac{d_u + d_v - 2}{d_ud_v}\right)^{1/2}$ over all edges $uv$ of $G$, where $d_u$ denotes the degree of a vertex $u$ of $G$. In this paper, we give the atom-bond connectivity index of the zigzag chain polyomino graphs. Meanwhile, we obtain the sharp upper bound on the atom-bond connectivity index of catacondensed polyomino graphs with $h$ squares and determine the corresponding extremal graphs.

1. Introduction

One of the most active fields of research in contemporary chemical graph theory is the study of topological indices (graph topological invariants) that can be used for describing and predicting physicochemical and pharmacological properties of organic compounds. In chemistry and for chemical graphs, these invariant numbers are known as the topological indices. There are many publications on the topological indices, see [1–6].

Polyomino graphs [13], also called chessboards [14] or square-cell configurations [15] have attracted some mathematicians’ considerable attention because many interesting combinatorial subjects are yielded from them such as domination problem and modeling problems of surface chemistry. A polyomino graph [16] is a connected geometric graph obtained by arranging congruent regular squares of side length 1 (called a cell) in a plane such that two squares are either disjoint or have a common edge. The polyomino graph has received considerable attentions.

Next, we introduce some graph definitions used in this paper.

Definition 1 (see [4]). Let $G$ be a polyomino graph. If all vertices of $G$ lie on its perimeter, then $G$ is said to be catacondensed polyomino graph or tree-like polyomino graph. (see Figure 1).

Definition 2 (see [16]). Let $G$ be a chain polyomino graph with $h$ squares. If the subgraph obtained from $G$ by deleting all the vertices of degree 2 and all the edges adjacent to the vertices is a path, then $G$ is said to be the zigzag chain polyomino graph, denoted by $Z_h$ (see Figure 1).

In this paper, we give the ABC indices of the zigzag chain polyomino graphs with $h$ squares and obtain the sharp upper
bound on the ABC indices of catacondensed polyomino graphs with \( h \) squares and determine the corresponding extremal graphs.

2. The ABC Indices of Catacondensed Polyomino Graphs

Let

\[
S_1 = \left\{ \sqrt{2} + \frac{2}{3}, \sqrt{2} + \frac{\sqrt{15}}{3} - \frac{2}{3}, \frac{\sqrt{2} + \sqrt{15}}{3} \right\},
\]

\[
S_2 = \left\{ 2, \frac{3\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3} - \frac{2}{3}, \frac{\sqrt{2} + \sqrt{15}}{3} \right\}.
\]

FIGURE 1: The zigzag chain polyomino graph \( Z_h \).

We call \( \sqrt{(d_u + d_v - 2)/d_u d_v} \) the weight of the edge \( uv \), denoted by \( W_{uv} \).

Note that for any catacondensed polyomino graph \( H^* \) with \( h \) squares, it can be obtained by gluing a new square \( s \) to some catacondensed polyomino graph \( H \) with \( h - 1 \) squares. So, we have the following lemma.

**Lemma 3.** Let \( H^* \) be a catacondensed polyomino graph with \( h \) squares which is obtained by gluing a new square \( s \) to some graph \( H \), where \( H \) is a catacondensed polyomino graph with \( h - 1 \) squares. One has

(i) If \( 2 \leq h \leq 3 \), then \( \text{ABC}(H^*) - \text{ABC}(H) \in S_1 \),

(ii) if \( h \geq 4 \), then \( \text{ABC}(H^*) - \text{ABC}(H) \in S_2 \).
Proof. Consider the following: (i) if $2 \leq h \leq 3$, by directly calculating, we have $ABC(H^*) - ABC(H) \in S_1$.

(ii) now, let $h \geq 4$. Without the loss of generality, let square $s$ be adjacent to the edge $AB$ in $H$ (see Figure 2). In the following, if the weights of some edges of $H$ have been changed when $s$ is adjacent to the edge $AB$ in $H$, then we marked these edges with thick lines in $H^*$. Let $D_i = ABC(H^*) - ABC(H) (i = 1, 2, \ldots, 35)$. Note that except the edge $AB$ of $s$, the summation of the weights of the remaining three edges is always $(3/2)\sqrt{2}$ in $H^*$. There are exactly three types of formations (see Figure 2).

Case 1. In Type I, $d_{A_1} = d_{B_1} = 2$ and $d_{A_2} = d_{B_2} = 3$ (see Figure 3).

By the definition of the ABC index, we have $ABC(H^*) - ABC(H) = (3/2)\sqrt{2} + (W_{A_1A} - W_{A_1B_1}) + (W_{A_2B_1} - W_{A_2B_2}) + (W_{B_1B_2} - W_{B_1B_2}) = D_i$ ($i = 1, 2, 3$).

If $d_u = 3$ and $d_v = 3$, then $D_1 = 2$.

If $d_u = 3$ and $d_v = 4$, or $d_u = 4$ and $d_v = 3$, then $D_2 = 4/3 + \sqrt{15}/6$.

If $d_u = 4$ and $d_v = 4$, then $D_3 = 2/3 + \sqrt{15}/3$.

Case 2. In Type II, $d_{A_1} = 2$, $d_{B_1} = 3$, $d_{A_2} = 3$, and $d_{B_2} = 4$ (see Figure 4).

Let $u$ adjacent to $A$ and $v, w$ adjacent to $B$ (see Figure 4).

Then $d_u \in \{2, 3, 4\}$, $d_v \in \{3, 4\}$, and $d_w \in \{2, 3, 4\}$. If $d_u = 2$, $d_v = 3$, and $d_w = 2$, which is in contradiction with $h \geq 4$; if $d_u = 3$ and $d_v = 3$, which is in contradiction with $d_{B_1} = 3$; if $d_u = 4$ and $d_v = 3$, which is in contradiction with $d_{A_1} = 2$ ($A \in V(H)$).

By the definition of the ABC index, we have $ABC(H^*) - ABC(H) = (3/2)\sqrt{2} + (W_{A_1A} - W_{A_1B_1}) + (W_{A_2B_1} - W_{A_2B_2}) + (W_{B_1B_2} - W_{B_1B_2}) + (W_{uB_2} - W_{wB_1}) = D_i$ ($i = 4, 5, \ldots, 14$).

Case 3. In Type III, $d_{A_1} = d_{B_1} = 3$ and $d_{A_2} = d_{B_2} = 4$ (see Figure 5).

Let $u, x$ adjacent to $A$ and $v, w$ adjacent to $B$ (see Figure 5).

Then, $d_u \in \{3, 4\}$, $d_v \in \{2, 3, 4\}$, and $d_w \in \{2, 3, 4\}$. Since the case $d_u = 3$, $d_v = 4$, $d_x = y_1$, and $d_w = y_2$ is the same as $d_u = 4$, $d_v = 3$, $d_x = y_2$, and $d_w = y_1$, where $y_1, y_2 \in [2, 4]$. And now that if $d_u = d_v = 3$ or $d_u = d_v = 4$, the vertices $x$ and $w$ are symmetric.

By the definition of the ABC index, we have $ABC(H^*) - ABC(H) = (3/2)\sqrt{2} + (W_{A_1A} - W_{A_1B_1}) + (W_{A_2B_1} - W_{A_2B_2}) + (W_{B_1B_2} - W_{B_1B_2}) + (W_{uB_2} - W_{wB_1}) = D_i$ ($i = 15, 16, \ldots, 35$).

If $d_u = d_v = 3$, $d_x = 2$, and $d_w = 3$, then $D_{15} = 3\sqrt{2}/2 + \sqrt{6}/4 + \sqrt{15}/2 - 8/3$.

If $d_u = d_v = 3$, $d_x = 2$, and $d_w = 4$, then $D_{16} = 3\sqrt{2}/2 + \sqrt{6}/4 + \sqrt{15}/2 - 10/3$.

If $d_u = d_v = 3$, $d_x = 3$, and $d_w = 3$, then $D_{17} = 3\sqrt{2}/2 + \sqrt{6}/4 + 2\sqrt{15}/3 - 10/3$.

If $d_u = d_v = 3$, $d_x = 3$, and $d_w = 4$, then $D_{18} = 3\sqrt{2}/2 + \sqrt{6}/4 + \sqrt{15}/3 - 8/3$.

If $d_u = d_v = 3$, $d_x = 4$, and $d_w = 4$, then $D_{19} = 3\sqrt{2}/2 + 3\sqrt{6}/4 - 2/3$.

If $d_u = d_v = 4$, $d_x = 2$, and $d_w = 2$, then $D_{20} = 3\sqrt{2}/2 + 3\sqrt{6}/4 - \sqrt{15}/3 - 2/3$.

If $d_u = d_v = 4$, $d_x = 2$, and $d_w = 3$, then $D_{21} = 3\sqrt{2}/2 + 3\sqrt{6}/4 - \sqrt{15}/6 - 4/3$.

If $d_u = d_v = 4$, $d_x = 2$, and $d_w = 4$, then $D_{22} = 3\sqrt{2}/2 + \sqrt{6} - \sqrt{15}/2 - 2/3$. 

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If \( d_u = d_v = 4, d_x = 3, \) and \( d_w = 3, \) then \( D_{23} = 3\sqrt{2}/2 + 3\sqrt{6}/4 - 2. \)

If \( d_u = d_v = 4, d_x = 3, \) and \( d_w = 4, \) then \( D_{24} = 3\sqrt{2}/2 + \sqrt{6} - \sqrt{15}/3 - 4/3. \)

If \( d_u = d_v = 4, d_x = 4, \) and \( d_w = 4, \) then \( D_{25} = 3\sqrt{2}/2 + 5\sqrt{6}/4 - 2\sqrt{15}/3 - 2/3. \)

If \( d_u = d_v = 4, d_x = 4, \) and \( d_w = 2, \) then \( D_{26} = 3\sqrt{2}/2 + \sqrt{6}/2 - 2/3. \)

If \( d_u = d_v = 4, d_x = 4, \) and \( d_w = 3, \) then \( D_{27} = 3\sqrt{2}/2 + \sqrt{6}/2 + \sqrt{15}/6 - 2. \)

If \( d_u = d_v = 4, d_x = 2, \) and \( d_w = 4, \) then \( D_{28} = 3\sqrt{2}/2 + 3\sqrt{6}/4 - \sqrt{15}/6 - 4/3. \)

If \( d_u = d_v = 4, d_x = 3, \) and \( d_w = 2, \) then \( D_{29} = 3\sqrt{2}/2 + \sqrt{6}/2 + \sqrt{15}/6 - 2. \)

If \( d_u = d_v = 4, d_x = 3, \) and \( d_w = 3, \) then \( D_{30} = 3\sqrt{2}/2 + \sqrt{6}/2 + \sqrt{15}/3 - 8/3. \)

If \( d_u = d_v = 4, d_x = 3, \) and \( d_w = 4, \) then \( D_{31} = 3\sqrt{2}/2 + 3\sqrt{6}/4 - 2. \)

If \( d_u = d_v = 4, d_x = 4, \) and \( d_w = 2, \) then \( D_{32} = 3\sqrt{2}/2 + 3\sqrt{6}/4 - \sqrt{15}/6 - 4/3. \)

If \( d_u = d_v = 4, d_x = 4, \) and \( d_w = 3, \) then \( D_{33} = 3\sqrt{2}/2 + 3\sqrt{6}/4 - 2. \)

If \( d_u = d_v = 4, d_x = 4, \) and \( d_w = 4, \) then \( D_{34} = 3\sqrt{2}/2 + \sqrt{6} - \sqrt{15}/3 - 4/3. \)

If \( d_u = d_v = 3, d_x = 3, \) and \( d_w = 2, \) then \( D_{35} = 3\sqrt{2}/2 + \sqrt{6}/4 + \sqrt{15}/3 - 2. \)

By directly calculating, we have \( i_0 = i_2, i_1 = i_3, \ldots, i_{34}, i_{35} = i_{30}, \) and \( i_{36} = i_{31} = i_{32} = i_{33}, \) \( i_{21} = i_{22} = i_{23} = i_{24} = i_{25}, \) and \( i_{26} = \max_{15 \leq i \leq 35} D_i, \) \( i_{27} = \min_{15 \leq i \leq 35} D_i. \) So \( ABC(H) - ABC(H) \in S^2, \) where \( h \geq 4. \)

Therefore, \( ABC(H^*) - ABC(H) \in S. \)

By Lemma 3, we have the following theorem.

\textbf{Theorem 4.} Let \( G \) be a catacondensed polyomino graph with \( h (h \geq 2) \) squares, then

\[
ABC(G) = 3\sqrt{2} + \frac{2}{3} + \left( \sqrt{2} + \frac{\sqrt{15}}{3} - \frac{2}{3} \right) a_1 + 2a_2 + \left( \frac{4}{3} + \frac{\sqrt{15}}{6} \right) a_3
\]

\[
+ \left( \frac{2}{3} + \frac{\sqrt{15}}{3} \right) a_4
\]

\[
+ \left( \sqrt{2} + \frac{\sqrt{15}}{2} - \frac{4}{3} \right) a_5
\]

\[
+ \left( \sqrt{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{6} - \frac{2}{3} \right) a_6
\]

\[
+ \left( \sqrt{2} + \frac{\sqrt{6}}{4} \right) a_7
\]

\[
+ \left( \sqrt{2} + \frac{\sqrt{6}}{2} - \frac{\sqrt{15}}{6} \right) a_8
\]

\[
+ \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{2}{3} \right) a_9
\]

\[
+ \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{6} \right) a_{10}
\]

\[
+ \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{2} + \frac{2}{3} - \frac{\sqrt{15}}{6} \right) a_{11}
\]

\[
+ \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3} - \frac{2}{3} \right) a_{12}
\]

\[
+ \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{2} \right) a_{13}
\]

\[
+ \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{2} - \frac{8}{3} \right) a_{14}
\]

\[
+ \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{2} + \frac{\sqrt{15}}{6} - \frac{2}{3} \right) a_{15}
\]

\[
+ \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{2\sqrt{15}}{3} - \frac{10}{3} \right) a_{16}
\]

\[
+ \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{2} + \frac{\sqrt{15}}{3} - \frac{8}{3} \right) a_{17}
\]

\[
+ \left( \frac{\sqrt{2}}{2} + \frac{3\sqrt{6}}{4} - \frac{2}{3} \right) a_{18}
\]

\[
+ \left( \frac{\sqrt{2}}{2} + \frac{3\sqrt{6}}{4} - \frac{\sqrt{15}}{3} - \frac{2}{3} \right) a_{19}
\]
where \( a_i \) is a nonnegative integer for \( i = 1, 2, \ldots, 25 \) and \( h = 2 + \sum_{i=1}^{25} a_i \).

Proof. We prove Theorem 4 by the induction on \( h \). If \( h = 2 \), by directly calculating, we have 

\[
ABC(G) = 3\sqrt{2} + \frac{2}{3} + \left( \sqrt{2} + \frac{\sqrt{15}}{3} - \frac{2}{3} \right) a_1
\]

\[+ 2a_2 + \left( \frac{4}{3} + \frac{\sqrt{15}}{6} \right) a_3 + \left( \frac{2}{3} + \frac{\sqrt{15}}{3} \right) a_4 + \left( \sqrt{2} + \frac{\sqrt{15}}{2} - \frac{4}{3} \right) a_5 + \left( \sqrt{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{6} - \frac{2}{3} \right) a_6 + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} \right) a_7 + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{2} - \frac{\sqrt{15}}{6} \right) a_8 + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{2}{3} \right) a_9 + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{6} \right) a_{10} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{2} + 2 \right) a_{11} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3} - \frac{2}{3} \right) a_{12} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3} - \frac{2}{3} \right) a_{13} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3} - \frac{2}{3} \right) a_{14} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3} - \frac{2}{3} \right) a_{15} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3} - \frac{2}{3} \right) a_{16} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3} - \frac{2}{3} \right) a_{17} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3} - \frac{2}{3} \right) a_{18} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3} - \frac{2}{3} \right) a_{19} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3} - \frac{2}{3} \right) a_{20} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3} - \frac{2}{3} \right) a_{21} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3} - \frac{2}{3} \right) a_{22} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3} - \frac{2}{3} \right) a_{23} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3} - \frac{2}{3} \right) a_{24} + \left( \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3} - \frac{2}{3} \right) a_{25},
\]

(3)

where \( a_i \) is a nonnegative integer for \( i = 1, 2, \ldots, 25 \) and \( h = 2 + \sum_{i=1}^{25} a_i \).

We will prove that Theorem 4 holds for \( h \) in the following. Let \( G^* \) be a catacondensed polyomino graph with \( h \) squares. Without the loss of generality, \( G^* \) can be obtained from some catacondensed polyomino graph \( G \) with \( h-1 \) squares by gluing a new square \( s \) to \( G \). By Lemma 3, we have 

\[
ABC(G^*) = ABC(G) + a
\]

\( \in S \). It means that 

\[
ABC(G^*) = ABC(G) + a
\]

where
There exists some \( l \in \{1, 2, \ldots, 25\} \) such that \( a_l^* = a_l + 1 \) and \( a_l^* = a_j \) for \( j \neq l \) (\( j \in \{1, 2, \ldots, 25\} \)). Obviously, \( a_i^* \) is a nonnegative integer for \( i = 1, 2, \ldots, 25 \) and 
\[
2 + \sum_{i=1}^{25} a_i^* = \sum_{i=1}^{25} a_i + 1 = h.
\]

**Lemma 5.** Let \( H \) be a catacondensed polyomino graph with \( h \) squares. If \( h \leq 3 \), there are exactly four nonisomorphism catacondensed polyomino graphs (see Figure 6), where \( ABC(H_1) = 2\sqrt{2} \), \( ABC(H_2) = 3\sqrt{2} + 2/3 \), \( ABC(H_3) = 3\sqrt{2} + 8/3 \), and \( ABC(H_4) = 4\sqrt{2} + \sqrt{15}/3 \).

**Theorem 6.** Let \( Z_h \) be a zigzag chain polyomino graph with \( h \) squares, then
\[
ABC(Z_h) = \begin{cases} 
2\sqrt{2}, & h = 1, \\
3\sqrt{2} + \frac{2}{3}, & h = 2, \\
(h + 1) \sqrt{2} + (h - 3) \cdot \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3}, & h \geq 3.
\end{cases}
\]

**Proof.** Obviously, \( Z_h \) can be obtained by gluing a new square \( s_h \) to \( Z_{h-1} \). Let \( s_{h-1} \) be the square adjacent to \( s_h \) (see Figure 1). We will prove Theorem 6 by the induction on \( h \).

If \( h = 1, 2, 3 \), then Theorem 6 holds (by Lemma 5). Assume that \( ABC(Z_{h-1}) = (h-1+1) \sqrt{2} + (h-1-3) \cdot (\sqrt{6}/4) + (\sqrt{15}/3) = h \sqrt{2} + (h-4) \cdot (\sqrt{6}/4) + (\sqrt{15}/3) \) for \( h - 1 \geq 3 \). By the induction assumption and the \( D_6 \) in Lemma 3, we have
\[
ABC(Z_h) = ABC(Z_{h-1}) + D_6
\]
\[
= h \sqrt{2} + (h-4) \cdot \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3} + \left( \sqrt{2} + \frac{\sqrt{6}}{4} \right)
\]
\[
= (h+1) \sqrt{2} + (h-3) \cdot \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3}.
\]
Note that $D_6 = \max_{1 \leq i \leq 35} D_i$ for $h \geq 4$ and by Lemma 5, we obtain the following Theorem 7.

**Theorem 7.** Let $G$ be a catacondensed polyomino graph with $h$ squares, then $ABC(G) \leq (h+1)\sqrt{2} + (h-3) \cdot (\sqrt{6}/4) + (\sqrt{15}/3)$, with the equality if and only if $G \cong Z_h$.

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**References**


