Hindawi Publishing Corporation
Discrete Dynamics in Nature and Society
Volume 2013, Article ID 598517, 7 pages
http://dx.doi.org/10.1155/2013/598517

Research Article

The Atom-Bond Connectivity Index of Catacondensed Polyomino Graphs

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Received 3 January 2013; Accepted 4 February 2013

Academic Editor: Zhengkun Huan

Let $G = (V, E)$ be a graph. The atom-bond connectivity (ABC) index is defined as the sum of weights $((d_u + d_v - 2)/d_u d_v)^{1/2}$ 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].

Let $G = (V, E)$ be a simple graph of order n. A few years ago, Estrada et al. [7] introduced a further vertex-degree-based graph invariant, known as the atom-bond connectivity (ABC) index. It is defined as:

$$\mathrm{ABC}(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}. \tag{1}$$

The ABC index keeps the spirit of the Randić index, and it provides a good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes [7]. Recently, the study of the ABC index attracts some research attention [6, 8–12].

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

$$
\begin{aligned}
S_1 &= \left\{\sqrt{2}+\frac{2}{3}, \sqrt{2}+\frac{\sqrt{15}}{3}-\frac{2}{3}, 2\right\},\\
S_2 &= \left\{2, \frac{3\sqrt{2}}{2}+\frac{\sqrt{6}}{4}+\frac{\sqrt{15}}{3}-2,\right.\\
&\qquad \frac{4}{3}+\frac{\sqrt{15}}{6}, \frac{2}{3}+\frac{\sqrt{15}}{3}, \sqrt{2}+\frac{\sqrt{15}}{3}-\frac{2}{3},\\
&\qquad \sqrt{2}+\frac{\sqrt{6}}{4}+\frac{\sqrt{15}}{6}-\frac{2}{3}, \sqrt{2}+\frac{\sqrt{6}}{4},\\
&\qquad \sqrt{2}+\frac{\sqrt{6}}{2}-\frac{\sqrt{15}}{6}, \frac{\sqrt{2}}{2}+\frac{\sqrt{6}}{4}+\frac{2}{3},\\
&\qquad \frac{\sqrt{2}}{2}+\frac{\sqrt{6}}{4}+\frac{\sqrt{15}}{6}, \frac{\sqrt{2}}{2}+\frac{\sqrt{6}}{2}+\frac{2}{3}-\frac{\sqrt{15}}{6},\\
&\qquad \frac{\sqrt{2}}{2}+\frac{\sqrt{6}}{4}+\frac{\sqrt{15}}{3}-\frac{2}{3}, \frac{\sqrt{2}}{2}+\frac{\sqrt{6}}{2},\\
&\qquad \frac{3\sqrt{2}}{2}+\frac{\sqrt{6}}{4}+\frac{\sqrt{15}}{2}-\frac{8}{3}, \frac{3\sqrt{2}}{2}+\frac{2\sqrt{6}}{4}+\frac{\sqrt{15}}{6}-2,\\
&\qquad \frac{3\sqrt{2}}{2}+\frac{\sqrt{6}}{4}+\frac{4\sqrt{15}}{6}-\frac{10}{3},\\
&\qquad \frac{3\sqrt{2}}{2}+\frac{\sqrt{6}}{2}+\frac{2\sqrt{15}}{6}-\frac{8}{3}, \frac{3\sqrt{2}}{2}+\frac{3\sqrt{6}}{4}-2,\\
&\qquad \frac{3\sqrt{2}}{2}+\frac{3\sqrt{6}}{4}-\frac{\sqrt{15}}{3}-\frac{2}{3}, \frac{3\sqrt{2}}{2}+\frac{3\sqrt{6}}{4}-\frac{\sqrt{15}}{6}-\frac{4}{3},\\
&\qquad \frac{3\sqrt{2}}{2}+\sqrt{6}-\frac{\sqrt{15}}{2}-\frac{2}{3}, \frac{3\sqrt{2}}{2}+\sqrt{6}-\frac{2\sqrt{15}}{6}-\frac{4}{3},\\
&\qquad \frac{3\sqrt{2}}{2}+\frac{5\sqrt{6}}{4}-\frac{2\sqrt{15}}{3}-\frac{2}{3},\\
&\qquad \left.\frac{3\sqrt{2}}{2}+\frac{\sqrt{6}}{2}-\frac{4}{3}, \frac{3\sqrt{2}}{2}+\frac{3\sqrt{6}}{4}+\frac{\sqrt{15}}{6}-\frac{8}{3}\right\},\\
S &= S_1 \bigcup S_2.
\end{aligned}
\tag{2}
$$

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.

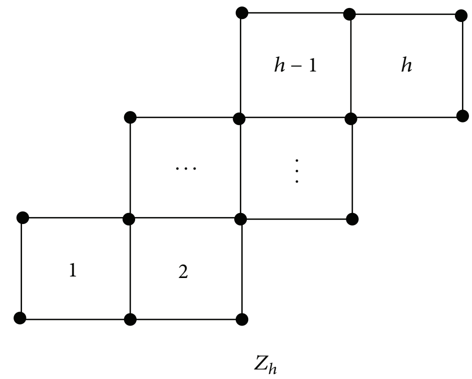

FIGURE 1: The zigzag chain polyomino graph Z_h.

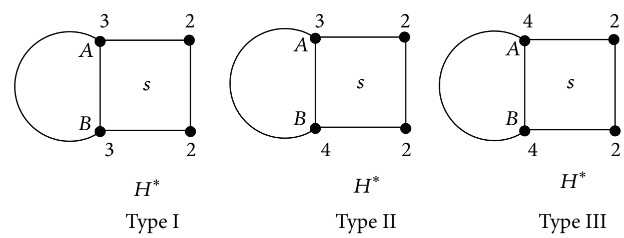

FIGURE 2

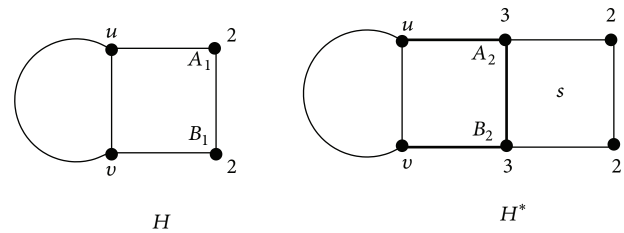

FIGURE 3

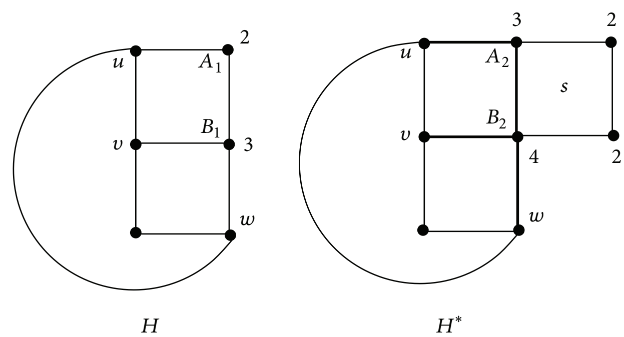

FIGURE 4

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* $2 \le h \le 3$, *then* $ABC(H^*) - ABC(H) \in S_1$,

(ii) *if* $h \ge 4$, *then* $ABC(H^*) - ABC(H) \in S_2$.

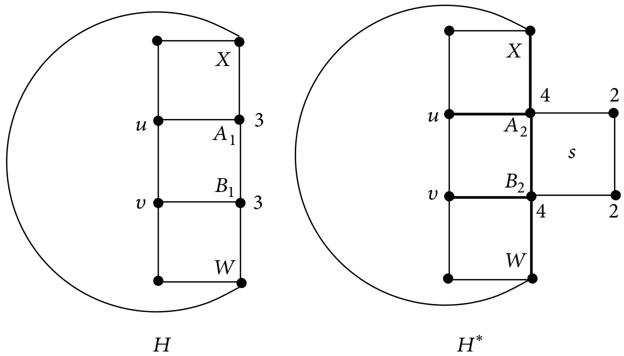

Figure 5

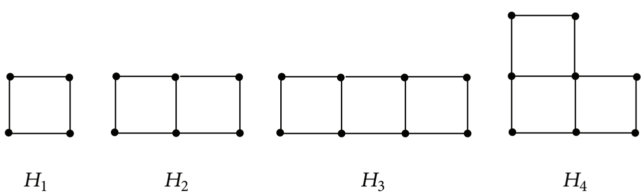

Figure 6: A catacondensed polyomino graph with h ($h \le 3$) squares.

Proof. Consider the following: (i) if $2 \le h \le 3$, by directly calculating, we have $\mathrm{ABC}(H^*) - \mathrm{ABC}(H) \in S_1$,

(ii) now, let $h \ge 4$. 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 $D_i = \mathrm{ABC}(H^*) - \mathrm{ABC}(H)$ ($i = 1, 2, \ldots, 35$). 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 ABC index, we have $\mathrm{ABC}(H^*) - \mathrm{ABC}(H) = (3/2)\sqrt{2} + (W_{uA_2} - W_{uA_1}) + (W_{A_2B_2} - W_{A_1B_1}) + (W_{vB_2} - W_{vB_1}) = D_i$ $(i = 1, 2, 3)$.

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 $h \ge 4$; 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 ABC index, we have $\mathrm{ABC}(H^*) - \mathrm{ABC}(H) = (3/2)\sqrt{2} + (W_{uA_2} - W_{uA_1}) + (W_{A_2B_2} - W_{A_1B_1}) + (W_{vB_2} - W_{vB_1}) + (W_{wB_2} - W_{wB_1}) = D_i$ $(i = 4, 5, \ldots, 14)$.

If $d_u = 2$, $d_v = 3$, and $d_w = 3$, then $D_4 = \sqrt{2} + \sqrt{15}/2 - 4/3$.

If $d_u = 2$, $d_v = 3$, and $d_w = 4$, then $D_5 = \sqrt{2} + \sqrt{6}/4 + \sqrt{15}/6 - 2/3$.

If $d_u = 2$, $d_v = 4$, and $d_w = 2$, then $D_6 = \sqrt{2} + \sqrt{6}/4$.

If $d_u = 2$, $d_v = 4$, and $d_w = 3$, then $D_7 = \sqrt{2} + \sqrt{6}/4 + \sqrt{15}/6 - 2/3$.

If $d_u = 2$, $d_v = 4$, and $d_w = 4$, then $D_8 = \sqrt{2} + \sqrt{6}/2 - \sqrt{15}/6$.

If $d_u = 3$, $d_v = 4$, and $d_w = 2$, then $D_9 = \sqrt{2}/2 + \sqrt{6}/4 + 2/3$.

If $d_u = 3$, $d_v = 4$, and $d_w = 3$, then $D_{10} = \sqrt{2}/2 + \sqrt{6}/4 + \sqrt{5/12}$.

If $d_u = 3$, $d_v = 4$, and $d_w = 4$, then $D_{11} = \sqrt{2}/2 + \sqrt{6}/2 + 2/3 - \sqrt{5/12}$.

If $d_u = 4$, $d_v = 4$, and $d_w = 2$, then $D_{12} = \sqrt{2}/2 + \sqrt{6}/4 + \sqrt{5/12}$.

If $d_u = 4$, $d_v = 4$, and $d_w = 3$, then $D_{13} = \sqrt{2}/2 + \sqrt{6}/4 + 2\sqrt{5/12} - 2/3$.

If $d_u = 4$, $d_v = 4$, and $d_w = 4$, then $D_{14} = \sqrt{2}/2 + \sqrt{6}/2$.

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, $d_u \in \{3,4\}$, $d_v \in \{3,4\}$, $d_w \in \{2,3,4\}$, and $d_x \in \{2,3,4\}$. 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 $y_1, y_2 \in \{2,3,4\}$. And note that if $d_u = d_v = 3$ or $d_u = d_v = 4$, the vertices x and w are symmetric.

By the definition of *ABC* index, we have $\mathrm{ABC}(H^*) - \mathrm{ABC}(H) = (3/2)\sqrt{2} + (W_{xA_2} - W_{xA_1}) + (W_{uA_2} - W_{uA_1}) + (W_{A_2B_2} - W_{A_1B_1}) + (W_{vB_2} - W_{vB_1}) + (W_{wB_2} - W_{wB_1}) = D_i$ $(i = 15, 16, \ldots, 35)$.

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 $D_{16} = 3\sqrt{2}/2 + \sqrt{6}/2 + \sqrt{15}/6 - 2$.

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 $D_{18} = 3\sqrt{2}/2 + \sqrt{6}/2 + \sqrt{15}/3 - 8/3$.

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

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 $D_{22} = 3\sqrt{2}/2 + \sqrt{6} - \sqrt{15}/2 - 2/3$.

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

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

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

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

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

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

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

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

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

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

By directly calculating, we have $D_5 = D_7$, $D_{10} = D_{12}$, $D_{16} = D_{27} = D_{29}$, $D_{18} = D_{30}$, $D_{19} = D_{23} = D_{31} = D_{33}$, $D_{21} = D_{28} = D_{32}$, $D_{24} = D_{34}$, and $D_6 = \max_{1\le i\le 35} D_i$, $D_{14} = \min_{1\le i\le 35} D_i$. So $\mathrm{ABC}(H^*) - \mathrm{ABC}(H) \in S_2$, where $h \ge 4$.

Therefore, $\mathrm{ABC}(H^*) - \mathrm{ABC}(H) \in S$. □

By Lemma 3, we have the following theorem.

Theorem 4. *Let G be a catacondensed polyomino graph with h ($h \ge 2$) squares, then*

$$\begin{aligned}
ABC(G) = {}& 3\sqrt{2} + \frac{2}{3} + \left(\sqrt{2} + \frac{\sqrt{15}}{3} - \frac{2}{3}\right) a_1 \\
& + 2a_2 + \left(\frac{4}{3} + \frac{\sqrt{15}}{6}\right) a_3 \\
& + \left(\frac{2}{3} + \frac{\sqrt{15}}{3}\right) a_4 \\
& + \left(\sqrt{2} + \frac{\sqrt{15}}{2} - \frac{4}{3}\right) a_5 \\
& + \left(\sqrt{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{6} - \frac{2}{3}\right) a_6 \\
& + \left(\sqrt{2} + \frac{\sqrt{6}}{4}\right) a_7 \\
& + \left(\sqrt{2} + \frac{\sqrt{6}}{2} - \frac{\sqrt{15}}{6}\right) a_8 \\
& + \left(\frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{2}{3}\right) a_9 \\
& + \left(\frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{6}\right) a_{10} \\
& + \left(\frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{2} + \frac{2}{3} - \frac{\sqrt{15}}{6}\right) a_{11} \\
& + \left(\frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3} - \frac{2}{3}\right) a_{12} \\
& + \left(\frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{2}\right) a_{13} \\
& + \left(\frac{3\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{2} - \frac{8}{3}\right) a_{14} \\
& + \left(\frac{3\sqrt{2}}{2} + \frac{\sqrt{6}}{2} + \frac{\sqrt{15}}{6} - 2\right) a_{15} \\
& + \left(\frac{3\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{2\sqrt{15}}{3} - \frac{10}{3}\right) a_{16} \\
& + \left(\frac{3\sqrt{2}}{2} + \frac{\sqrt{6}}{2} + \frac{\sqrt{15}}{3} - \frac{8}{3}\right) a_{17} \\
& + \left(\frac{3\sqrt{2}}{2} + \frac{3\sqrt{6}}{4} - 2\right) a_{18} \\
& + \left(\frac{3\sqrt{2}}{2} + \frac{3\sqrt{6}}{4} - \frac{\sqrt{15}}{3} - \frac{2}{3}\right) a_{19}
\end{aligned}$$

$$+\left(\frac{3\sqrt{2}}{2}+\frac{3\sqrt{6}}{4}-\frac{\sqrt{15}}{6}-\frac{4}{3}\right)a_{20}$$
$$+\left(\frac{3\sqrt{2}}{2}+\sqrt{6}-\frac{\sqrt{15}}{2}-\frac{2}{3}\right)a_{21}$$
$$+\left(\frac{3\sqrt{2}}{2}+\sqrt{6}-\frac{\sqrt{15}}{3}-\frac{4}{3}\right)a_{22}$$
$$+\left(\frac{3\sqrt{2}}{2}+\frac{5\sqrt{6}}{4}-\frac{2\sqrt{15}}{3}-\frac{2}{3}\right)a_{23}$$
$$+\left(\frac{3\sqrt{2}}{2}+\frac{\sqrt{6}}{2}-\frac{4}{3}\right)a_{24}$$
$$+\left(\frac{3\sqrt{2}}{2}+\frac{\sqrt{6}}{4}+\frac{\sqrt{15}}{3}-2\right)a_{25}, \tag{3}$$

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 $\mathrm{ABC}(G) = 3\sqrt{2} + 2/3$, where $a_i = 0$ $(i = 1, 2, \ldots, 25)$. So, Theorem 4 holds for $h = 2$.

Assume that Theorem 4 holds for all catacondensed polyomino graphs with $h - 1$ $(h - 1 \geq 2)$ squares, that is,

$$\mathrm{ABC}(G) = 3\sqrt{2}+\frac{2}{3}+\left(\sqrt{2}+\frac{\sqrt{15}}{3}-\frac{2}{3}\right)a_1$$
$$+2a_2+\left(\frac{4}{3}+\frac{\sqrt{15}}{6}\right)a_3$$
$$+\left(\frac{2}{3}+\frac{\sqrt{15}}{3}\right)a_4$$
$$+\left(\sqrt{2}+\frac{\sqrt{15}}{2}-\frac{4}{3}\right)a_5$$
$$+\left(\sqrt{2}+\frac{\sqrt{6}}{4}+\frac{\sqrt{15}}{6}-\frac{2}{3}\right)a_6$$
$$+\left(\sqrt{2}+\frac{\sqrt{6}}{4}\right)a_7$$
$$+\left(\sqrt{2}+\frac{\sqrt{6}}{2}-\frac{\sqrt{15}}{6}\right)a_8$$
$$+\left(\frac{\sqrt{2}}{2}+\frac{\sqrt{6}}{4}+\frac{2}{3}\right)a_9$$
$$+\left(\frac{\sqrt{2}}{2}+\frac{\sqrt{6}}{4}+\frac{\sqrt{15}}{6}\right)a_{10}$$
$$+\left(\frac{\sqrt{2}}{2}+\frac{\sqrt{6}}{2}+\frac{2}{3}-\frac{\sqrt{15}}{6}\right)a_{11}$$
$$+\left(\frac{\sqrt{2}}{2}+\frac{\sqrt{6}}{4}+\frac{\sqrt{15}}{3}-\frac{2}{3}\right)a_{12}$$
$$+\left(\frac{\sqrt{2}}{2}+\frac{\sqrt{6}}{2}\right)a_{13}$$
$$+\left(\frac{3\sqrt{2}}{2}+\frac{\sqrt{6}}{4}+\frac{\sqrt{15}}{2}-\frac{8}{3}\right)a_{14}$$
$$+\left(\frac{3\sqrt{2}}{2}+\frac{\sqrt{6}}{2}+\frac{\sqrt{15}}{6}-2\right)a_{15}$$
$$+\left(\frac{3\sqrt{2}}{2}+\frac{\sqrt{6}}{4}+\frac{2\sqrt{15}}{3}-\frac{10}{3}\right)a_{16}$$
$$+\left(\frac{3\sqrt{2}}{2}+\frac{\sqrt{6}}{2}+\frac{\sqrt{15}}{3}-\frac{8}{3}\right)a_{17}$$
$$+\left(\frac{3\sqrt{2}}{2}+\frac{3\sqrt{6}}{4}-2\right)a_{18}$$
$$+\left(\frac{3\sqrt{2}}{2}+\frac{3\sqrt{6}}{4}-\frac{\sqrt{15}}{3}-\frac{2}{3}\right)a_{19}$$
$$+\left(\frac{3\sqrt{2}}{2}+\frac{3\sqrt{6}}{4}-\frac{\sqrt{15}}{6}-\frac{4}{3}\right)a_{20}$$
$$+\left(\frac{3\sqrt{2}}{2}+\sqrt{6}-\frac{\sqrt{15}}{2}-\frac{2}{3}\right)a_{21}$$
$$+\left(\frac{3\sqrt{2}}{2}+\sqrt{6}-\frac{\sqrt{15}}{3}-\frac{4}{3}\right)a_{22}$$
$$+\left(\frac{3\sqrt{2}}{2}+\frac{5\sqrt{6}}{4}-\frac{2\sqrt{15}}{3}-\frac{2}{3}\right)a_{23}$$
$$+\left(\frac{3\sqrt{2}}{2}+\frac{\sqrt{6}}{2}-\frac{4}{3}\right)a_{24}$$
$$+\left(\frac{3\sqrt{2}}{2}+\frac{\sqrt{6}}{4}+\frac{\sqrt{15}}{3}-2\right)a_{25}, \tag{4}$$

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

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 $\mathrm{ABC}(G^*) - \mathrm{ABC}(G) \in S$. It means that $\mathrm{ABC}(G^*) = \mathrm{ABC}(G) + a$, where

$a \in S$. By the induction assumption and direct computation, we have

$$\begin{aligned}
\mathrm{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{3\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{2} - \frac{8}{3}\right) a_{14}^* \\
&+ \left(\frac{3\sqrt{2}}{2} + \frac{\sqrt{6}}{2} + \frac{\sqrt{15}}{6} - 2\right) a_{15}^* \\
&+ \left(\frac{3\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{2\sqrt{15}}{3} - \frac{10}{3}\right) a_{16}^* \\
&+ \left(\frac{3\sqrt{2}}{2} + \frac{\sqrt{6}}{2} + \frac{\sqrt{15}}{3} - \frac{8}{3}\right) a_{17}^* \\
&+ \left(\frac{3\sqrt{2}}{2} + \frac{3\sqrt{6}}{4} - 2\right) a_{18}^* \\
&+ \left(\frac{3\sqrt{2}}{2} + \frac{3\sqrt{6}}{4} - \frac{\sqrt{15}}{3} - \frac{2}{3}\right) a_{19}^* \\
&+ \left(\frac{3\sqrt{2}}{2} + \frac{3\sqrt{6}}{4} - \frac{\sqrt{15}}{6} - \frac{4}{3}\right) a_{20}^* \\
&+ \left(\frac{3\sqrt{2}}{2} + \sqrt{6} - \frac{\sqrt{15}}{2} - \frac{2}{3}\right) a_{21}^* \\
&+ \left(\frac{3\sqrt{2}}{2} + \sqrt{6} - \frac{\sqrt{15}}{3} - \frac{4}{3}\right) a_{22}^* \\
&+ \left(\frac{3\sqrt{2}}{2} + \frac{5\sqrt{6}}{4} - \frac{2\sqrt{15}}{3} - \frac{2}{3}\right) a_{23}^* \\
&+ \left(\frac{3\sqrt{2}}{2} + \frac{\sqrt{6}}{2} - \frac{4}{3}\right) a_{24}^* \\
&+ \left(\frac{3\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3} - 2\right) a_{25}^*.
\end{aligned} \tag{5}$$

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

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 $ABC(H_1) = 2\sqrt{2}$, $ABC(H_2) = 3\sqrt{2} + 2/3$, $ABC(H_3) = 3\sqrt{2} + 8/3$, $ABC(H_4) = 4\sqrt{2} + \sqrt{15}/3$.*

Theorem 6. *Let Z_h be a zigzag chain polyomino graph with h squares, then*

$$ABC(Z_h) = \begin{cases} 2\sqrt{2}, & h = 1, \\ 3\sqrt{2} + \dfrac{2}{3}, & h = 2, \\ (h+1)\sqrt{2} + (h-3) \cdot \dfrac{\sqrt{6}}{4} + \dfrac{\sqrt{15}}{3}, & h \geq 3. \end{cases} \tag{6}$$

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 $\mathrm{ABC}(Z_{h-1}) = (h-1+1)\sqrt{2} + (h-1-3)\cdot(\sqrt{6}/4) + (\sqrt{15}/3) = h\sqrt{2} + (h-4)\cdot(\sqrt{6}/4) + (\sqrt{15}/3)$ for $h - 1 \geq 3$. By the induction assumption and the D_6 in Lemma 3, we have

$$\begin{aligned}
\mathrm{ABC}(Z_h) &= \mathrm{ABC}(Z_{h-1}) + D_6 \\
&= h\sqrt{2} + (h-4)\cdot\frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3} + \left(\sqrt{2} + \frac{\sqrt{6}}{4}\right) \\
&= (h+1)\sqrt{2} + (h-3)\cdot\frac{\sqrt{6}}{4} + \frac{\sqrt{15}}{3}.
\end{aligned} \tag{7}$$

So, Theorem 6 holds. □

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 $G \cong Z_h$.*

Acknowledgments

The project was supported by NSFC (no. 11071272; 11101086; 11101087) and the Foundation of Fuzhou University (no. 2012-XQ-30).

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