Double hexagonal chains with the extremal PI indices *

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Abstract

The Padmakar-Ivan (PI) index of a graph $G = (V, E)$ is defined as $PI(G) = \sum_{e \in E}(n_{eu}(e|G) + n_{ev}(e|G))$, where $e = uv$, $n_{eu}(e|G)$ is the number of edges of G lying closer to u than to v and $n_{ev}(e|G)$ is the number of edges of G lying closer to v than to u. In this paper, we give a recursive formula for computing the PI index of a double hexagonal chain by using the orthogonal cut, and characterize the double hexagonal chains with the extremal PI indices.

1 Introduction

The numbers reflecting certain structural features of organic molecules that are obtained from the molecular graph are usually called graph invariants or more commonly topological indices. One of the oldest molecular graph-based structural descriptor of organic molecule is the Wiener index or Wiener number [1], this quantity is equal to the sum of distances between all pairs of vertices of the respective molecular graph. Since then, many topological indices have been designed [2]. Such a proliferation is still going on and is becoming counter productive. In 1990s, Gutman [3] and coworkers [4] introduced a generalization of the Wiener index (W) for cyclic graphs called Szeged index (Sz). The main advantage of the Szeged index is that it is a modification of W; otherwise, it coincides with the Wiener index. In [5,6] another topological index was introduced and it was

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named Padmakar-Ivan index, abbreviated as PI. The PI index of a graph G is defined as:

$$PI(G) = \sum_{e \in E(G)} [n_{eu}(e|G) + n_{ev}(e|G)] \tag{1}$$

where $e = uv$, $n_{eu}(e|G)$ is the number of edges of G lying closer to u than v, $n_{ev}(e|G)$ is the number of edges of G lying closer to v than u and summation goes over all edges of G. The edges equidistant from u and v are not considered for the calculation of PI index. Since PI index is different for acyclic graphs, several applications of PI index are reported in the literature [13-20].

Recently, [7] gave the formulas for calculating the PI indices of catacondensed hexagonal systems, and characterized the extremal catacondensed hexagonal systems with the minimum or maximum PI index. [8-11] computed the PI indices of $TUVC_6[2p, q]$, zig-zag polyhex nanotubes, the torus covering by C_4 and C_8 and the nanotube covering by C_4 and C_8. [12] described a method of computing PI index of benzenoid hydrocarbons using orthogonal cuts. The method requires the finding of number of edges in the orthogonal cuts in a benzenoid system. In this paper, we give a recursive formula for computing the PI index of a double hexagonal chain and characterize the double hexagonal chains with the extremal PI indices using this method.

A hexagonal system is a 2-connected plane graph whose every interior face is bounded by a regular hexagon of unit length 1. Hexagonal systems are of considerable importance in theoretical chemistry because they are the natural graph representation of benzenoid hydrocarbons [1]. A vertex of a hexagonal system belongs to, at most, three hexagons. A vertex shared by three hexagons is called an internal vertex of the respective hexagonal system. A hexagonal system H is said to be catacondensed if it does not possess internal vertices, otherwise H is said to be pericondensed. A hexagonal chain is a catacondensed hexagonal system which has no hexagon adjacent to more than two hexagons. An k-tuple hexagonal chain consists of k condensed identical hexagonal chains. When $k = 2$, we call it a double hexagonal chain [1-2].

A double hexagonal chain can be constructed inductively. Let us orient the naphthalene so that its interior edges are horizontal. There are two types of fusion of two naphthalenes: (i) $b \equiv r$, $c \equiv s$, $d \equiv t$, $e \equiv u$; (ii) $a \equiv s$, $b \equiv t$, $c \equiv u$, $d \equiv v$ as shown in Figure 1. We call them α-type and β-type fusing, respectively. Any double hexagonal chain can be obtained from a naphthalene B by a stepwise fusion of new naphthalene, and at each step a type of fusion is selected from θ-type fusing, where $\theta \in \{\alpha, \beta\}$.

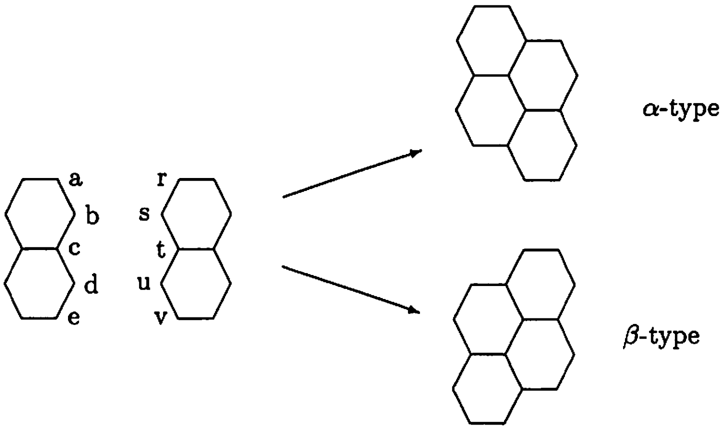

Figure 1. α-type fusing, β-type fusing.

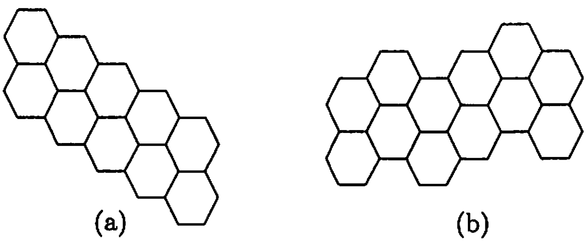

Figure 2. (a) $B(\alpha, \alpha, \alpha, \alpha)$; (b) $B(\beta, \alpha, \beta, \beta, \alpha)$.

Let $B(\theta_1, \theta_2, \cdots, \theta_n)$ be the double hexagonal chain with $2(n+1)$ hexagons obtained from a naphthalene B by θ_1-type, θ_2-type, $\cdots$, θ_n-type, successively. And $B(\alpha, \alpha, \cdots, \alpha)$ or $B(\beta, \beta, \cdots, \beta)$ is called the double linear hexagonal chain (see Figure 2).

Let

$$\overline{\theta} = \begin{cases} \beta, & \text{if } \theta = \alpha; \\ \alpha, & \text{if } \theta = \beta. \end{cases}$$

Then $B(\theta_1, \theta_2, \cdots, \theta_n) \cong B(\overline{\theta_1}, \overline{\theta_2}, \cdots, \overline{\theta_n})$. If $n \geq 1$, the double hexagonal chain $B(\theta_1, \theta_2, \cdots, \theta_n)$ is a pericondensed hexagonal system.

2 Calculation of the PI index of a double hexagonal chain from orthogonal cuts

Let $G = (V, E)$ be the embedding of a connected, planar and bipartite graph in the Euclidean plane; $V = V(G)$ and $E = E(G)$ are the vertex and the edge set of G, respectively. The number of edges of G is denoted by $m = m(G) = |E|$.

Let $d(x, y)$ denote the length of a shortest path connecting vertices $x, y \in V$. $e' = u'v' \in E$ is called strongly codistant to $e = uv \in E$ (briefly: e' sco e) if and only if $d(u, u') = d(v, v') = d$ and $d(u, v') = d(v, u') = d + 1$, or vice versa, and $d \geq 0$. An orthogonal cut $C(e)$ with respect to e is the set of all edges $e' \in E$, which are strongly codistant to e ([12]):

$$C(e) = \{e' \in E | e' \text{ is strongly codistant to e}\}.$$

The relation sco is an equivalence relation on the edge set E of a bipartite graph G, and the orthogonal cut $C(e)$ is the equivalence class containing e.

For a bipartite graph G, the edge set $E = E(G)$ is the union of pairwise disjoint equivalence classes of orthogonal cuts $C_j = C_j(G)$, $j = 1, 2, \cdots, k$, of graph G. Let $m_j = |C_j|$ be the number of edges of orthogonal cut C_j. Then, it is showed in [12] that the equation (1) is now

$$PI(G) = m^2 - \sum_{j=1}^{k} m_j^2. \tag{2}$$

In the following, we give a recursive formula for computing the PI index of a double hexagonal chain $B(\theta_1, \theta_2, \cdots, \theta_n)$. Since $B(\theta_1, \theta_2, \cdots, \theta_n)$ is isomorphic to $B(\overline{\theta_1}, \overline{\theta_2}, \cdots, \overline{\theta_n})$, we always assume that $\theta_n = \alpha$.

Note that the number of edges in $B(\theta_1, \theta_2, \cdots, \theta_n)$ is $11 + 8n$. As in Figure 3, except $C_0, C_1, C_2, C_1', C_2'$, the other orthogonal cuts of $B(\theta_1, \theta_2, \cdots, \theta_n)$ are the same of $B(\theta_1, \theta_2, \cdots, \theta_{n-1})$. From (2), we have

$$
\begin{aligned}
& PI(B(\theta_1,\theta_2,\cdots,\theta_n)) - PI(B(\theta_1,\theta_2,\cdots,\theta_{n-1})) \\
= \; & 128n + 112 - |C_0|^2 - |C_1|^2 - |C_2|^2 - |C_1'|^2 - |C_2'|^2 \\
& +(|C_1|-1)^2 + (|C_2|-1)^2 + (|C_2'|-1)^2 \\
= \; & 128n + 102 - 2(|C_1| + |C_2| + |C_2'|) \\
= \; & 128n + 102 - 2(x+y+z)
\end{aligned}
$$

where $x = |C_1|$, $y = |C_2|$, $z = |C_2'|$, and x, y, z are dependent on $\theta_1, \theta_2, \cdots, \theta_n$.

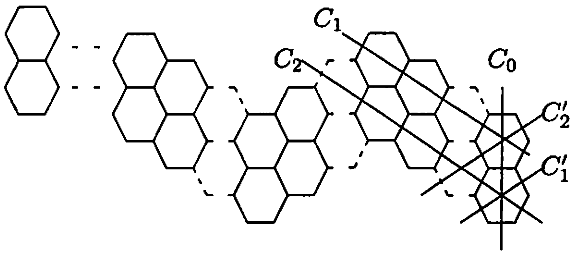

Figure 3. The other orthogonal cuts $C_0, C_1, C_2, C_1', C_2'$.

Let $(\theta_n, \theta_{n-1}, \cdots, \theta_1) = (\underbrace{\alpha,\cdots,\alpha}_{r_1}, \underbrace{\beta,\cdots,\beta}_{r_2}, \underbrace{\alpha,\cdots,\alpha}_{r_3}, \beta, \cdots)$, where

$$
\begin{cases}
r_1 + r_2 + r_3 \le n \\
1 \le r_1 \le n \\
0 \le r_2 \le n - r_1 \\
r_2 = 0 \text{ if and only if } r_1 = n \\
0 \le r_3 \le n - r_1 - r_2 \\
r_2 \ge 1 \text{ if } r_3 \ge 1.
\end{cases}
\tag{3}
$$

(I) $r_1 = n$. Then, both of C_1 and C_2 pass through $r_1 + 1$ hexagons, C_2' passes two hexagons. And $x = y = r_1 + 2 = n + 2$, $z = 3$.

(II) $r_1 = 1$. Then, C_1 passes two hexagons, C_2' passes $r_2 + 2$ hexagons. And $x = 3$, $z = r_2 + 3$.

When $r_2 = 1$, C_2 passes $r_3 + 3$ hexagons and $y = r_3 + 4$;

When $r_2 \ge 2$, C_2 passes three hexagons and $y = 4$.

(III) $1 < r_1 < n$. Then, C_1 passes $r_1 + 1$ hexagons, C_2' passes two hexagons. And $x = r_1 + 2$, $z = 3$.

When $r_2 = 1$, C_2 passes $r_3 + r_1 + 2$ hexagons and $y = r_3 + r_1 + 3$;

When $r_2 \ge 2$, C_2 passes $r_1 + 2$ hexagons and $y = r_1 + 3$.

So,

$$x+y+z=\begin{cases} 2n+7, & r_1=n; \\ 2r_1+r_3+8, & 1<r_1<n \text{ and } r_2=1; \\ 2r_1+7, & 1<r_1<n \text{ and } r_2\geq 2; \\ r_3+11, & r_1=1 \text{ and } r_2=1; \\ r_2+10, & r_1=1 \text{ and } r_2\geq 2. \end{cases}$$

And we have the following recursive formula

Theorem 1. Let $(\theta_n,\theta_{n-1},\cdots,\theta_1)=(\underbrace{\alpha,\cdots,\alpha}_{r_1},\underbrace{\beta,\cdots,\beta}_{r_2},\underbrace{\alpha,\cdots,\alpha}_{r_3},\beta,\cdots)$.

Then

$$PI(B(\theta_1,\theta_2,\cdots,\theta_n))=PI(B(\theta_1,\theta_2,\cdots,\theta_{n-1})) + \begin{cases} 124n+88, & r_1=n; \\ 128n+86-4r_1-2r_3, & 1<r_1<n \text{ and } r_2=1; \\ 128n+88-4r_1, & 1<r_1<n \text{ and } r_2\geq 2; \\ 128n+80-2r_3, & r_1=1 \text{ and } r_2=1; \\ 128n+82-2r_2, & r_1=1 \text{ and } r_2\geq 2. \end{cases}$$

3 Extremal double hexagonal chains with respect to the PI index

Using Theorem 1 and $PI(B)=96$, we can compute out:

If $n=1$, then $PI(B(\theta))=308$.

If $n=2$, then $PI(B(\theta_1,\theta_2))=644$.

If $n=3$, then

$$PI(B(\theta_1,\theta_2,\theta_3))=\begin{cases} PI(B(\alpha,\alpha,\alpha))=1104; \\ PI(B(\beta,\alpha,\alpha))=1106; \\ PI(B(\alpha,\beta,\alpha))=1106; \\ PI(B(\beta,\beta,\alpha))=1106. \end{cases}$$

If $n=4$, then

$$PI(B(\theta_1,\theta_2,\theta_3,\theta_4))=\begin{cases} PI(B(\alpha,\alpha,\alpha,\alpha))=1688; \\ PI(B(\beta,\alpha,\alpha,\alpha))=1692; \\ PI(B(\alpha,\beta,\alpha,\alpha))=1694; \\ PI(B(\beta,\beta,\alpha,\alpha))=1698; \\ PI(B(\alpha,\alpha,\beta,\alpha))=1694; \\ PI(B(\beta,\alpha,\beta,\alpha))=1696; \\ PI(B(\alpha,\beta,\beta,\alpha))=1696; \\ PI(B(\beta,\beta,\beta,\alpha))=1694. \end{cases}$$

Theorem 2. $PI(B(\theta_1,\theta_2,\cdots,\theta_n))\geq 62n^2+150n+96$ with the equality if and only if $\theta_1=\cdots=\theta_n=\alpha$ or $\theta_1=\cdots=\theta_n=\beta$.

Proof. Since $B(\theta_1,\theta_2,\cdots,\theta_n)\cong B(\overline{\theta_1},\overline{\theta_2},\cdots,\overline{\theta_n})$, we may assume that $\theta_n=\alpha$.

It is easy to see that the result holds for $0\le n\le 4$.

Suppose that the result is true for $n-1$. We show that the result holds for $n\ge 5$.

By Theorem 1, we have

$$\begin{aligned}PI(B(\underbrace{\alpha,\cdots,\alpha}_{n})) &= PI(B(\underbrace{\alpha,\cdots,\alpha}_{n-1}))+124n+88\\ &= PI(B)+124(1+2+\cdots+n)+88n\\ &= 62n^2+150n+96\end{aligned}$$

and

$$0<\begin{cases}4n-2-4r_1-2r_3, & 1<r_1<n \text{ and } r_2=1;\\ 4n-4r_1, & 1<r_1<n \text{ and } r_2\ge 2;\\ 4n-8-2r_3, & r_1=1 \text{ and } r_2=1;\\ 4n-6-2r_2, & r_1=1 \text{ and } r_2\ge 2.\end{cases}$$

since $r_1+r_2+r_3\le n$. So,

$$PI(B(\theta_1,\theta_2,\cdots,\theta_n))\ge PI(B(\theta_1,\theta_2,\cdots,\theta_{n-1}))+124n+88$$

with the equality if and only if $r_1=n$ from (3). Thus the result holds for $n\ge 0$.

The proof of Theorem 2 is complete.

Theorem 3. Let $n\ge 1$. Then

$$PI(B(\theta_1,\theta_2,\cdots,\theta_n))\le\begin{cases}64n^2+143n+102, & \text{if } n \text{ is even;}\\ 64n^2+143n+101, & \text{if } n \text{ is odd}\end{cases}$$

with the equality if and only if $(\theta_1,\cdots,\theta_n)=(\alpha,\alpha,\beta,\beta,\cdots)$ or $(\beta,\beta,\alpha,\alpha,\cdots)$ for even $n\ge 4$, and $(\theta_1,\cdots,\theta_n)=(\alpha,\alpha,\beta,\beta,\cdots)$ or $(\beta,\beta,\alpha,\alpha,\cdots)$ or $(\beta,\alpha,\alpha,\beta,\beta,\cdots)$ or $(\alpha,\beta,\beta,\alpha,\alpha,\cdots)$ for odd $n\ge 5$.

Proof. Since $B(\theta_1,\theta_2,\cdots,\theta_n)\cong B(\overline{\theta_1},\overline{\theta_2},\cdots,\overline{\theta_n})$, we may assume that $\theta_n=\alpha$.

We use the inductive method on n. It can be seen that the result holds for $n=1,2,3,4,5$ by computing immediately from the recursive formula in Theorem 1.

Let $n \geq 6$ and $(\theta_n, \theta_{n-1}, \cdots, \theta_1) = (\underbrace{\alpha, \cdots, \alpha}_{r}, \underbrace{\beta, \cdots, \beta}_{s}, \underbrace{\alpha, \cdots, \alpha}_{t}, \underbrace{\beta, \cdots, \beta}_{k}, \alpha, \cdots)$. By Theorem 1, we have

$$\begin{aligned} & PI(B(\theta_1, \theta_2, \cdots, \theta_n)) \\ = \; & PI(B(\theta_1, \theta_2, \cdots, \theta_{n-1})) + \Delta_1 \\ = \; & PI(B(\theta_1, \theta_2, \cdots, \theta_{n-2})) + \Delta_2 + \Delta_1. \end{aligned}$$

(i) If $r = n$, then

$\Delta_2 + \Delta_1 = 124(n-1) + 88 + 124n + 88 < 128(n-1) + 128n + 78 + 80.$

(ii) If $1 < r < n$ and $s = 1$, then $\Delta_1 = 128n + 86 - 4r - 2t$,

$$\Delta_2 = \begin{cases} 128(n-1) + 86 - 4(r-1) - 2t, & \text{if } 2 < r < n; \\ 128(n-1) + 80 - 2t, & \text{if } r = 2 \end{cases}$$

and $\Delta_2 + \Delta_1 \leq 128(n-1) + 128n + 78 + 80$ with the equality if and only if $r = 2$ and $t = 0$.

(ii) If $1 < r < n$ and $s \geq 2$, then $\Delta_1 = 128n + 88 - 4r$,

$$\Delta_2 = \begin{cases} 128(n-1) + 88 - 4(r-1), & \text{if } 2 < r < n; \\ 128(n-1) + 82 - 2s, & \text{if } r = 2 \end{cases}$$

and $\Delta_2 + \Delta_1 \leq 128(n-1) + 128n + 78 + 80$ with the equality if and only if $r = s = 2$.

(iv) If $r = 1$ and $s = 1$, then $\Delta_1 = 128n + 80 - 2t$,

$$\Delta_2 = \begin{cases} 128(n-1) + 80 - 2k, & \text{if } t = 1; \\ 128(n-1) + 82 - 2t, & \text{if } t \geq 2 \end{cases}$$

and $\Delta_2 + \Delta_1 \leq 128(n-1) + 128n + 78 + 80$ with the equality if and only if $t = 1$ and $k = 0$.

(v) If $r = 1$ and $s \geq 2$, then $\Delta_1 = 128n + 82 - 2s$,

$$\Delta_2 = \begin{cases} 124(n-1) + 88, & \text{if } s = n-1; \\ 128(n-1) + 86 - 4s - 2k, & \text{if } 1 < s < n-1 \text{ and } t = 1; \\ 128(n-1) + 88 - 4s, & \text{if } 1 < s < n-1 \text{ and } t \geq 2 \end{cases}$$

and $\Delta_2 + \Delta_1 \leq 128(n-1) + 128n + 78 + 80$ with the equality if and only if $s = 2$ and $t \geq 2$.

Hence,

$$PI(B(\theta_1, \theta_2, \cdots, \theta_n)) \leq PI(B(\theta_1, \theta_2, \cdots, \theta_{n-2})) + 128(n-1) + 128n + 78 + 80$$

with the equality if and only if $r = s = 2$ or $r = 1, s = 2, t \geq 2$.

By the inductive hypotheses,

$$PI(B(\theta_1, \theta_2, \cdots, \theta_{n-2})) \leq \begin{cases} 64(n-2)^2 + 143(n-2) + 102, & \text{if } n \text{ is even;} \\ 64(n-2)^2 + 143(n-2) + 101, & \text{if } n \text{ is odd} \end{cases}$$

with the equality if and only if $(\theta_1, \cdots, \theta_{n-2}) = (\alpha, \alpha, \beta, \beta, \cdots)$ or $(\theta_1, \cdots, \theta_{n-2}) = (\beta, \beta, \alpha, \alpha, \cdots)$ for even $n \geq 6$, and $(\theta_1, \cdots, \theta_{n-2}) = (\alpha, \alpha, \beta, \beta, \cdots)$ or $(\beta, \beta, \alpha, \alpha, \cdots)$ or $(\beta, \alpha, \alpha, \beta, \beta, \cdots)$ or $(\alpha, \beta, \beta, \alpha, \alpha, \cdots)$ for odd $n \geq 7$.

So,

$$PI(B(\theta_1, \theta_2, \cdots, \theta_n)) \leq \begin{cases} 64n^2 + 143n + 102, & \text{if } n \text{ is even;} \\ 64n^2 + 143n + 101, & \text{if } n \text{ is odd} \end{cases}$$

with the equality if and only if $(\theta_1, \cdots, \theta_n) = (\alpha, \alpha, \beta, \beta, \cdots)$ or $(\beta, \beta, \alpha, \alpha, \cdots)$ for even $n \geq 4$, and $(\theta_1, \cdots, \theta_n) = (\alpha, \alpha, \beta, \beta, \cdots)$ or $(\beta, \beta, \alpha, \alpha, \cdots)$ or $(\beta, \alpha, \alpha, \beta, \beta, \cdots)$ or $(\alpha, \beta, \beta, \alpha, \alpha, \cdots)$ for odd $n \geq 5$.

The proof of Theorem 3 is complete.

4 Conclusion

Let $T(\theta_1, \theta_2, \cdots, \theta_n)$ be a k-tuple hexagonal chain constructed inductively as the double hexagonal chains. The number of its edges is $(3k+2)n + (5k+1)$. We hope to get a recursive formula for computing the PI index of $T(\theta_1, \theta_2, \cdots, \theta_n)$ by using the orthogonal cut, and we can also get

$$\begin{aligned} & PI(T(\theta_1, \theta_2, \cdots, \theta_n)) - PI(T(\theta_1, \theta_2, \cdots, \theta_{n-1})) \\ = \; & (2n-1)(3k+2)^2 + 2(5k+1)(3k+2) \\ & -(|C_0|^2 + |C_1|^2 + \cdots + |C_k|^2 + |C_1'|^2 + \cdots + |C_k'|^2) \\ & +(|C_1| - 1)^2 + \cdots + (|C_k| - 1)^2 + (|C_2'| - 1)^2 + \cdots + (|C_k'| - 1)^2 \\ = \; & (2n-1)(3k+2)^2 + 2(5k+1)(3k+2) - (k+1)^2 - 4 + (2k-1) \\ & -2(|C_1| + \cdots + |C_k| + |C_2'| + \cdots + |C_k'|) \end{aligned}$$

Where $|C_0| = k+1$ and $|C_1'| = 2$. When we try to compute $|C_i|$ and $|C_j'|$, we find that they are dependent on $\theta_1, \theta_2, \cdots, \theta_n$. In fact, if

$$(\theta_n, \theta_{n-1}, \cdots, \theta_1) = (\underbrace{\alpha, \cdots, \alpha}_{r_1}, \underbrace{\beta, \cdots, \beta}_{r_2}, \underbrace{\alpha, \cdots, \alpha}_{r_3}, \beta, \cdots),$$

then $|C_k|$ and $|C_k'|$ are dependent on $r_1, r_2, \cdots, r_{k+1}$. So, the more k is large, the more it becomes complicated. It needs a new method to get a recursive formula for computing the PI index of the k-tuple hexagonal chains.

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