On Spanning Trees in Catacondensed Molecules

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Among all catacondensed benzenoid molecules the unbranched systems possess the largest number of spanning trees. Some other relations for the spanning-tree count of catacondensed benzenoids are also reported. The results obtained continue to hold for catacondensed molecules composed of rings the size of which differ from six. The propositions reported do, however, depend for their validity on there being rings of only one size in the catacondensed system under study.

Introduction

Interest in the enumeration of spanning trees in graphs [1, 2] – originally accomplished by Kirchhoff [3] in the context of electrical networks nearly a century and a half ago – has, in recent years, been renewed [4–15]. This revival has been both practical [8, 9, 14, 15] (for example, at the microscopic level, in connection with the calculation of π-electron "ring-currents" in conjugated systems, in which the concept of spanning tree is of relevance [9]) and mathematical [4–7, 10–13] (extending the classic "Matrix-Tree" theorem [2], thereby leading to devices [5–7, 10–13] that give ever-more efficient ways of counting spanning trees). These new methods [10–13] have already been applied [14, 15] to establish the "complexity" of (i.e., the number of spanning trees in) systems such as the topical buckminsterfullerene [14, 15], in which the spanning-tree count is of the order of 10^{20}.

In this paper, we offer a largely mathematical analysis of the complexity of catacondensed benzenoid hydrocarbons and, amongst other results, we show that, of such molecules, the unbranched systems possess the largest number of spanning trees. The propositions that we prove are also valid for catacondensed molecules comprising rings of size other than six; our results do, though, depend on there being rings of *only one size* in the catacondensed system under study.

If **G** is a labelled (molecular) graph then any connected acyclic subgraph of **G**, containing all the vertices of **G**, is called a spanning tree of **G**. For instance, the molecular graph of anthracene and two of its spanning trees are depicted below.
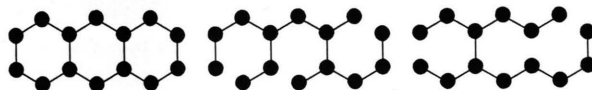
The number of distinct spanning trees of a labelled graph **G** is denoted by $t(\mathbf{G})$. In the case of polycyclic molecular graphs $t(\mathbf{G})$ is usually very large. For example, the anthracene graph has a total of 204 spanning trees. As already mentioned, the t-values of the fullerenes are of the order of 10^{20} [14, 15].

Enumerating the Spanning Trees in Catacondensed Molecules

A polycyclic molecule is called catacondensed if its rings have either one chemical bond in common or are disjoint, and if no three rings share a common atom. In this paper we are interested exclusively in those catacondensed molecules all rings of which are of equal size. By far the best known such molecules belong to the class of benzenoid systems [16]; their rings are of size six.

The molecular graphs $\mathbf{G}_1$, $\mathbf{G}_2$, $\mathbf{G}_3$, and $\mathbf{G}_4$ represent catacondensed benzenoid hydrocarbons. The molecular graph $\mathbf{G}_5$ is an example of a non-benzenoid catacondensed species with (unique) ring size 8.

G_1

G_2

G_3

G_4

G_5

The inner dual of a catacondensed molecule is the graph the vertices of which correspond to the rings of this molecule, and these vertices are adjacent only if the respective rings share a chemical bond. The following example is self-explanatory: $ID(G_6)$ is the inner dual of the molecular graph G_6.

G_6 $ID(G_6)$
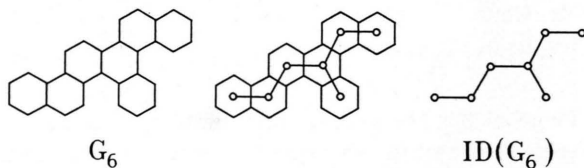
Note that the inner dual is a simple graph which does not purport to give any *geometrical* information; the angles between its edges are, therefore, arbitrary and are a matter of convention. This, in particular, means that non-isomorphic catacondensed systems may have isomorphic inner-duals. For example, the inner dual of the molecular graph G_3 is identical to $ID(G_6)$. Similarly, $ID(G_1) = ID(G_2)$.

$ID(G_1)$ $ID(G_2)$ $ID(G_3)$

$ID(G_4)$ $ID(G_5)$
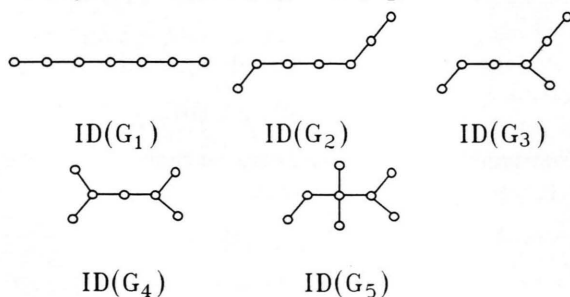
As should be evident from the above examples, the inner dual of a catacondensed molecule is a connected, acyclic graph – i.e., a tree. The maximum vertex degree of the inner dual of a catacondensed molecule is at most $r/2$ (if r is even) and $(r-1)/2$ (if r is odd), where r stands for the size of the rings. For benzenoid molecules $r = 6$, which means that the largest vertex degrees encountered in the inner duals of these kinds of molecules are either 3 (e.g., in $ID(G_3)$, $ID(G_4)$ and $ID(G_6)$) or 2 (e.g., in $ID(G_1)$ and $ID(G_2)$). The maximum vertex degree of $ID(G_5)$ is 4, which is in harmony with the fact that G_5 is composed of 8-membered rings, $r = 8$.

In [10] the following remarkable and surprising result was obtained, that enables easy enumeration of the spanning trees for certain molecular graphs:

$$t(G) = \phi(ID(G), r) \tag{1}$$

where $\phi(H, x)$ stands for the characteristic polynomial [2] of the graph H and r is the (unique) size of the rings in the molecule considered; for benzenoids, $r = 6$.

For instance, the characteristic polynomials of the inner duals of G_5 and G_6 are [2]

$$\phi(ID(G_5), x) = x^8 - 7x^6 + 11x^4 - 4x^2,$$

$$\phi(ID(G_6), x) = x^7 - 6x^5 + 9x^3 - 3x.$$

Therefore, G_5 and G_6 possess $8^8 - 7 \cdot 8^6 + 11 \cdot 8^4 - 4 \cdot 8^2 = 14\,987\,008$ and $6^7 - 6 \cdot 6^5 + 9 \cdot 6^3 - 3 \cdot 6 = 235\,206$ spanning trees, respectively.

Some Inequalities for the Characteristic Polynomials of Trees

According to formula (1), the information about the number of spanning trees of a catacondensed molecule is contained in the characteristic polynomial of its inner dual. This inner dual, on the other hand, is a tree. In this section, we establish certain relations between the characteristic polynomials of trees which, by means of (1), imply inequalities between the spanning-tree counts of the respective catacondensed molecules. In order to do this, we first recall a few well-known results from graph-spectral theory [2].

Let $\phi(G) = \phi(G, x)$ denote the characteristic polynomial of the graph G. Further, let $\Lambda(G)$ be the largest eigenvalue of G, i.e., the largest root of the equation $\phi(G, x) = 0$.

$1°$: If d_{max} is the maximum vertex degree of a graph G, then $\Lambda(G) \le d_{max}$. This, in particular, means that

$\phi(\mathbf{G}, x)$ is greater than zero for all values of the variable x, $x > d_{max}$.

Observe that the quantity r in (1) certainly satisfies the condition $r > d_{max}$.

2°: If $\mathbf{H}$ is a subgraph of the graph $\mathbf{G}$, then $\Lambda(\mathbf{H}) \le \Lambda(\mathbf{G})$.

An edge $\mathbf{e}$ of a graph $\mathbf{G}$ is called a *bridge* if $\mathbf{G} - \mathbf{e}$ has more components than $\mathbf{G}$. All edges of acyclic graphs are bridges.

3°: If $\mathbf{e}$ is a bridge of the graph $\mathbf{G}$, connecting the vertices $\mathbf{u}$ and $\mathbf{v}$, then

$$\phi(\mathbf{G}) = \phi(\mathbf{G} - \mathbf{e}) - \phi(\mathbf{G} - \mathbf{u} - \mathbf{v}). \tag{2}$$

All edges of a tree are bridges. Consequently, if $\mathbf{G}$ is a tree then (2) is applicable to any of its edges.

4°: Let $\mathbf{G} \cup \mathbf{H}$ symbolise the union of disjoint graphs $\mathbf{G}$ and $\mathbf{H}$. Then

$$\phi(\mathbf{G} \cup \mathbf{H}) = \phi(\mathbf{G}) \cdot \phi(\mathbf{H}). \tag{3}$$

Note that (3) is also true if $\mathbf{H}$ is the empty graph (i.e., the graph without vertices or edges): in this case, $\mathbf{G} \cup \mathbf{H} = \mathbf{G}$ and $\phi(\mathbf{H}) = 1$.

The tree containing only two vertices of degree one is called a path. The path with n vertices is denoted by $\mathbf{P}_n$. For instance, $\mathbf{ID}(\mathbf{G}_1)$ and $\mathbf{ID}(\mathbf{G}_2)$ are isomorphic to $\mathbf{P}_7$.

In 1973, Lovász and Pelikán [17] proved the following theorem.

5°: Let $\mathbf{T}$ be a tree with n vertices, different from $\mathbf{P}_n$. If $x > \Lambda(\mathbf{P}_n)$, then

$$\phi(\mathbf{P}_n, x) > \phi(\mathbf{T}, x). \tag{4}$$

Because of 1° the relation (4) certainly holds for $x = r$. Therefore, when the Lovász-Pelikán theorem is combined with formula (1) we see that the unbranched catacondensed molecules always have more spanning trees than their branched isomers.

We now report what may be regarded as a generalisation of the Lovász-Pelikán formula.

Let $\mathbf{T}$ be an arbitrary tree and $\mathbf{v}$ an arbitrary vertex within it. Then by $\mathbf{T}[i]\,\mathbf{P}_n$ we denote the tree obtained by identifying the i-th vertex of the path $\mathbf{P}_n$ with the vertex $\mathbf{v}$ of $\mathbf{T}$:

$$\mathbf{P}_n \qquad\qquad \mathbf{T}[i]\mathbf{P}_n$$
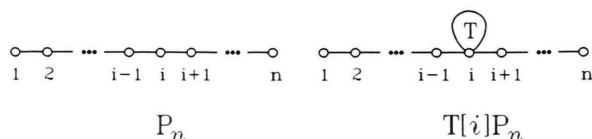
6°: Let $k = \text{int}(n/2)$. Then, for all values of x such that $x > \max\{\Lambda(\mathbf{T}[i]\,\mathbf{P}_n) \mid i = 1, 2, \ldots, k\}$,

$$\phi(\mathbf{T}[1]\,\mathbf{P}_n) > \phi(\mathbf{T}[2]\,\mathbf{P}_n) > \ldots > \phi(\mathbf{T}[k]\,\mathbf{P}_n). \tag{5}$$

In order to prove the relations (5) we need the following two auxiliary results, namely 7° and 8°.

7°: Let $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_j$ be edges of the tree $\mathbf{T}$. Then, for all values of x such that $x > \Lambda(\mathbf{T})$,

$$\phi(\mathbf{T} - \mathbf{e}_1 - \mathbf{e}_2 - \ldots - \mathbf{e}_j) > \phi(\mathbf{T}). \tag{6}$$

8°: Let $k = \text{int}(n/2)$. Then, for all values of x such that $x > \phi(\mathbf{P}_n)$, $\tag{7}$

$$\Lambda(\mathbf{P}_n) < \phi(\mathbf{P}_{n-1} \cup \mathbf{P}_1) < \phi(\mathbf{P}_{n-2} \cup \mathbf{P}_2) < \ldots < \phi(\mathbf{P}_{n-k} \cup \mathbf{P}_k).$$

Proof of 7°: We first demonstrate the validity of (6) for $j = 1$. Let the edge $\mathbf{e}_1$ connect the vertices $\mathbf{u}_1$ and $\mathbf{v}_1$. If $x > \Lambda(\mathbf{T})$ then, because of property 2°, $x > \Lambda(\mathbf{T} - \mathbf{e}_1)$ and $x > \Lambda(\mathbf{T} - \mathbf{u}_1 - \mathbf{v}_1)$. Whence, all three characteristic polynomials $\phi(\mathbf{T})$, $\phi(\mathbf{T} - \mathbf{e}_1)$ and $\phi(\mathbf{T} - \mathbf{u}_1 - \mathbf{v}_1)$ are positive-valued for $x > \Lambda(\mathbf{T})$. Bearing in mind (2), i.e.,

$$\phi(\mathbf{T}) = \phi(\mathbf{T} - \mathbf{e}_1) - \phi(\mathbf{T} - \mathbf{u}_1 - \mathbf{v}_1),$$

we now easily conclude that $\phi(\mathbf{T}) < \phi(\mathbf{T} - \mathbf{e}_1)$.

Repeating the same argument we arrive at $\phi(\mathbf{T} - \mathbf{e}_1) < \phi(\mathbf{T} - \mathbf{e}_1 - \mathbf{e}_2)$, $\phi(\mathbf{T} - \mathbf{e}_1 - \mathbf{e}_2) < \phi(\mathbf{T} - \mathbf{e}_1 - \mathbf{e}_2 - \mathbf{e}_3)$, etc. Continued application of this process ultimately results in the inequality (6).

Proof of 8°: The first relation in (7) is, of course, a special case of (6). In order to verify the remaining relations it is sufficient to prove that, for $j < k$,

$$\phi(\mathbf{P}_{n-j} \cup \mathbf{P}_j) < \phi(\mathbf{P}_{n-j-1} \cup \mathbf{P}_{j+1}). \tag{8}$$

Applying (2) to edges $(j, j+1)$ and $(j+1, j+2)$ we obtain

$$\phi(\mathbf{P}_n) = \phi(\mathbf{P}_j \cup \mathbf{P}_{n-j}) - \phi(\mathbf{P}_{j-1} \cup \mathbf{P}_{n-j-1})$$
$$= \phi(\mathbf{P}_{j+1} \cup \mathbf{P}_{n-j-1}) - \phi(\mathbf{P}_j \cup \mathbf{P}_{n-j-2}),$$

thus

$$\phi(\mathbf{P}_{n-j} \cup \mathbf{P}_j) - \phi(\mathbf{P}_{n-j-1} \cup \mathbf{P}_{j+1})$$
$$= \phi(\mathbf{P}_{n-j-1} \cup \mathbf{P}_{j-1}) - \phi(\mathbf{P}_{n-j-2} \cup \mathbf{P}_j).$$

Continuing the same argument we conclude that the relation

$$\phi(\mathbf{P}_{n-j} \cup \mathbf{P}_j) - \phi(\mathbf{P}_{n-j-1} \cup \mathbf{P}_{j+1})$$
$$= \phi(\mathbf{P}_{n-j-h} \cup \mathbf{P}_{j-h}) - \phi(\mathbf{P}_{n-j-1-h} \cup \mathbf{P}_{j+1-h})$$

holds for all $h = 1, 2, \ldots, j$. Choosing $h = j$ we obtain

$$\phi(\mathbf{P}_{n-j} \cup \mathbf{P}_j) - \phi(\mathbf{P}_{n-j-1} \cup \mathbf{P}_{j+1})$$
$$= -[\phi(\mathbf{P}_1 \cup \mathbf{P}_{n-2j-1}) - \phi(\mathbf{P}_{n-2j})].$$

As a special case of (2),

$$\phi(\mathbf{P}_{n-2j}) = \phi(\mathbf{P}_1 \cup \mathbf{P}_{n-2j-1}) - \phi(\mathbf{P}_{n-2j-2})$$

which, combined with the previous result, yields the remarkable identity (9)

$$\phi(\mathbf{P}_{n-j} \cup \mathbf{P}_j) - \phi(\mathbf{P}_{n-j-1} \cup \mathbf{P}_{j+1}) = -\phi(\mathbf{P}_{n-2j-2}). \quad (9)$$

For $x > \varLambda(\mathbf{P}_n)$, the characteristic polynomial of $\mathbf{P}_{n-2j-2}$ is certainly positive-valued. Whence, the right-hand side of (9) is negative-valued and the inequality (8) follows.

This completes the proof of property 8°.

Proof of 6°: Suppose that the vertex $\mathbf{v}$ of the tree $\mathbf{T}$ in formula (5) has degree d and that the edges incident to it are $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_d$. Then the tree $\mathbf{T}$ has the structure depicted below.

T
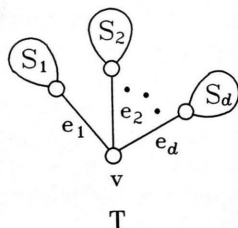
If the edges $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_d$ are deleted from $\mathbf{T}$ then the rest decomposes into $d+1$ components, namely, an isolated vertex ($\mathbf{v}$) and the trees $\mathbf{S}_1, \mathbf{S}_2, \ldots, \mathbf{S}_d$.

Now, by applying the relation (2) successively to the edges $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_d$ of the compound graph $\mathbf{T}[i]\,\mathbf{P}_n$, we obtain

$$\phi(\mathbf{T}[i]\,\mathbf{P}_n) = \phi(\mathbf{P}_n \cup \mathbf{S}_1 \cup \mathbf{S}_2 \cup \ldots \cup \mathbf{S}_d)$$
$$- \phi(\mathbf{P}_{i-1} \cup \mathbf{P}_{n-i} \cup \mathbf{S}_1' \cup \mathbf{S}_2 \cup \ldots \cup \mathbf{S}_d)$$
$$- \phi(\mathbf{P}_{i-1} \cup \mathbf{P}_{n-i} \cup \mathbf{S}_1 \cup \mathbf{S}_2' \cup \ldots \cup \mathbf{S}_d) - \ldots$$
$$- \phi(\mathbf{P}_{i-1} \cup \mathbf{P}_{n-i} \cup \mathbf{S}_1 \cup \mathbf{S}_2 \cup \ldots \cup \mathbf{S}_d'),$$

where $\mathbf{S}_j'$ is the graph obtained from $\mathbf{S}_j$ by deleting the end-vertex of the edge $\mathbf{e}_j$. Bearing in mind property 4°, we may write the above formula as

$$\phi(\mathbf{T}[i]\,\mathbf{P}_n) = \{\phi(\mathbf{P}_n)\,\phi(\mathbf{S}_1 \cup \mathbf{S}_2 \cup \ldots \cup \mathbf{S}_d)\}$$
$$- \phi(\mathbf{P}_{i-1} \cup \mathbf{P}_{n-i})\,\{\phi(\mathbf{S}_1' \cup \mathbf{S}_2 \cup \ldots \cup \mathbf{S}_d)$$
$$+ \phi(\mathbf{S}_1 \cup \mathbf{S}_2' \cup \ldots \cup \mathbf{S}_d) + \ldots$$
$$+ \phi(\mathbf{S}_1 \cup \mathbf{S}_2 \cup \ldots \cup \mathbf{S}_d')\} \quad (10)$$

where the terms in braces are independent of the position of the tree $\mathbf{T}$ in $\mathbf{T}[i]\,\mathbf{P}_n$, i.e., are independent of the parameter i. The requirement $x > \max\{\varLambda(\mathbf{T}[i]\,\mathbf{P}_n)\,|\,i = 1, 2, \ldots, k\}$ guarantees that all polynomials on the right-hand side of (10) are positive-valued. Then $\phi(\mathbf{T}[i]\,\mathbf{P}_n)$ monotonically decreases as the quantity $\phi(\mathbf{P}_{i-1} \cup \mathbf{P}_{n-i})$ increases. Property 6° now follows from property 8°.

5° follows from 6°. In order to show that, for x being sufficiently large, the Lovász-Pelikán inequality (4) is a consequence of the relations (5), notice that the maximum value of $\phi(\mathbf{T}[i]\,\mathbf{P}_n)$ is achieved when $i = 1$. If $i \neq 1$, then the i-th vertex in $\mathbf{T}[i]\,\mathbf{P}_n$ has degree $d + 2$. If, however, $i = 1$, then the degree of this vertex is $d + 1$. Whence, $\mathbf{T}[1]\,\mathbf{P}_n$ is always less branched than $\mathbf{T}[i]\,\mathbf{P}_n$, $i \neq 1$. In other words, the transformation $\mathbf{T}[i]\,\mathbf{P}_n \to \mathbf{T}[1]\,\mathbf{P}_n$ always reduces the extent of branching, but increases the value of the characteristic polynomial.

If $\mathbf{T}[1]\,\mathbf{P}_n$ is not isomorphic to the path-graph, then it can be viewed as a tree of the form $\mathbf{T}^*[j]\,\mathbf{P}_{n^*}$, with $j \neq 1$. Then the transformation $\mathbf{T}^*[j]\,\mathbf{P}_{n^*} \to \mathbf{T}^*[1]\,\mathbf{P}_{n^*}$ will again reduce the extent of branching and at the same time increase the value of the characteristic polynomial.

Repeating such transformations a sufficient number of times ultimately yields the unbranched tree = path, the characteristic polynomial of which is thus maximal.

This is not a complete demonstration of the validity of the Lovász-Pelikán theorem 4° because, throughout our considerations, we have assumed that the variable x is "sufficiently large" – i.e., larger than the maximum vertex degree of any graph involved in the proof. This, however, causes no difficulty as long as we are concerned with the enumeration of spanning trees via (1). As already pointed out, the value $x = r$ in (1) exceeds $d_{\max}$ it is at least twice as big.

Applications to Spanning Trees

When the results of the previous section are combined with formula (1) we immediately reach the following conclusions.
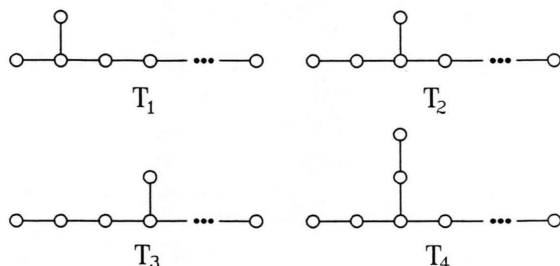
Proposition 0. Catacondensed molecules having equal ring sizes and isomorphic inner-duals have the same number of spanning trees.

Proposition 1. Among all catacondensed molecules with a given number of rings and given ring sizes, unbranched systems have maximum numbers of spanning trees.

Proposition 2. The larger the extent of branching of the catacondensed molecule, the smaller is its spanning-tree count.

Proposition 3. The closer the branching point is to the end of the chain, the larger is the number of spanning trees that the molecule possesses.

Let T_1, T_2, T_3, and T_4 be n-vertex trees of the following structure.

Let $C[T]$ be an n-cyclic catacondensed molecular-graph the inner dual of which is T. Then the following specialisations of Propositions 1–3 can be deduced. In what follows, the ring-size, r, is assumed to be fixed.

Proposition 4. (a) For all n-cyclic catacondensed systems C, $n \geq 4$, $t(C) \leq t(C[P_n])$.

(b) For all n-cyclic catacondensed systems C, $n \geq 5$, different from $C[P_n]$, $t(C) \leq t(C[T_1])$.

(c) For all n-cyclic catacondensed systems C, $n \geq 6$, different from $C[P_n]$ and $C[T_1]$, $t(C) \leq t(C[T_2])$.

(d) For all n-cyclic catacondensed systems C, $n \geq 7$, different from $C[P_n]$, $C[T_1]$, and $C[T_2]$, $t(C) \leq t(C[T_3])$.

(e) For all n-cyclic catacondensed systems C, $n \geq 7$, different from $C[P_n]$, $C[T_1]$, $C[T_2]$, and $C[T_3]$, $t(C) \leq t(C[T_4])$.

Concluding Remarks

Many other relations of this kind could be established using the above-described graph-spectral reasoning. Whilst primarily, in this paper, the emphasis is on deducing general and mathematically exact results, we draw attention to a further *chemical* implication of the complexity of a graph representing a *molecule*, that arises in the context of chemical nomenclature [15]. It has been pointed out [15] that any notation for a given molecule and its derivatives involves selecting what amounts to a spanning tree of the molecule, in order to label its vertices and thus to produce the required linear notation [18]. The complexity is some measure of the ease of identifying and comparing derivatives on such an indexing scheme. The main motivation for this work, though, has been to establish that unbranched systems are the catacondensed benzenoid hydrocarbons with the largest number of spanning trees and to initiate investigation of how far these ideas may be extended to analogous (non-benzenoid) structures comprising only r-membered rings, when

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