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Growth in [*n*]helicenes

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The generating function of the sequence that represents the number of graph vertices at a given distance from the root is called the spherical growth function of the rooted graph. This mathematical notion is first applied to finite and infinite graphs representing [*n*]helicenes, the simplest nonplanar unbranched catacondensed benzenoid hydrocarbons. The calculation of growth function is then generalized to graphs that have an arbitrary connected graph in place of each hexagon and therefore represent a subclass of fasciagraphs. Also, the connection between the growth function of a finite graph and its Wiener index is established.

INTRODUCTION

A polyhex is a graph consisting of congruent hexagons, where two hexagons either share exactly one edge or are disjoint.[1] A simply connected polyhex represents the carbon skeleton of a benzenoid hydrocarbon and is either called a benzenoid graph or a helicene graph depending on whether it is geometrically planar or nonplanar, respectively.[2] In each case we consider only graphs which represent benzenoid molecules without holes, therefore excluding coronoids.[3]

A benzenoid graph is also known as a benzenoid system, a hexagonal system and even as a polyhex.[4] If all vertices of a benzenoid graph G lie on its perimeter, *i.e.*, on the boundary, then G is said to be catacondensed, otherwise it is pericondensed.[5] Catacondensed benzenoid graphs have two types of vertices; the ones of degree 2 that belong to only one hexagon, and the ones of degree 3 that lie on exactly two adjacent hexagons. The same is true for nonplanar catacondensed polyhexes also known as catacondensed helicene graphs.[6] In general, helicenes can include other aromatic compounds besides benzene but we consider only [*n*]helicenes[7] (also called helixes)[8] made up of *n* angularly rotated benzene rings producing helically shaped molecules.

Recall the definition of growth in rooted graphs.[9] Let G be a connected, finite or locally finite graph (infinite but with finite vertex degrees) and let V(G) be the set of vertices of G. The distance $d(u,v)$ between two vertices u and v equals the number of edges in a shortest path between vertices u and v in G. By selecting a vertex $r \in$ G we define the (spherical) growth sequence as $\{\delta(\mathrm{G},r,i) \mid i = 0,1,2,...\}$, where $\delta(\mathrm{G},r,i)$ denotes the number of vertices at a distance i from r. By taking the generating function[10] for $\delta(\mathrm{G},r,i)$ we get the growth function (called also the growth) of graph G rooted at r:

$$\Delta(\mathrm{G},r;\, x) = \sum_{i=0}^{\infty} \delta(\mathrm{G},r,i)\, x^i.$$

The vertex r, upon which the growth function depends, is called the root. We can extend the definition by

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allowing a root to be any induced subgraph R of the graph G, where the distance between a vertex $u \in$ G and the root R is defined as $d(u,\mathrm{R}) = \min_{r\in \mathrm{V(R)}}\{d(u,r)\}$. In particular, the expression $\delta(\mathrm{G,R},0)$ equals the number of vertices in R. Two root types are of a special importance. If a root is a vertex, it is known as a vertex root and if it consists of two adjacent vertices, it is called an edge root.

In our paper about the growth in catacondensed benzenoid graphs[11] we presented an algorithm to calculate the growth recursively. In this paper we apply the methods from[11] on to the set of graphs representing [n]helicenes that are the simplest form of helicenes. Their unbranched helicoidal structure allows us to write the growth in a compact form for finite and infinite (but locally finite) graphs. The distinction between one-way and two-way infinite [n]helicenes is made by denoting them [∞]helicenes and [$\pm\infty$]helicenes, respectively.

We also show how the algorithm,[11] used to calculate the growth of [∞]helicene graphs, can be generalized to a subclass of fasciagraphs,[12] where the hexagon representing each benzene ring is substituted with an arbitrary graph. A fasciagraph $\gamma_m(\mathrm{G};X)$ is obtained from a line graph of length m by replacing each vertex with an arbitrary graph G and each edge with a set of edges $\mathrm{X} \subseteq \mathrm{V(G)} \times \mathrm{V(G)}$. If we start with a cycle instead of a line graph, we get a structure known as a rotagraph.

THE WIENER INDEX AND THE GROWTH FUNCTION

The Wiener index is one of many distance-based topological indices and has many uses in chemistry. It has been studied thoroughly in the literature; generally[13,14] or specific to catacondensed benzenoids,[15,16] hexagonal chains[17] and fasciagraphs.[18] For an arbitrary finite graph G its Wiener index is defined as the sum of the distances between all unordered pairs of its vertices. It can be written as

$$W(\mathrm{G}) = \sum_{\{u,v\}\subseteq \mathrm{V(G)}} d(u,v).$$

The Wiener index of a graph G can also be calculated with the help of the growth functions of the graph.

Proposition 1

$$W(\mathrm{G}) = \frac{1}{2}\sum_{v\in \mathrm{V(G)}} \Delta'(\mathrm{G},v;1). \qquad (1)$$

Proof: Since $\Delta'(\mathrm{G},v;1)$ sums the distances from v to all other vertices and the summation over all vertices of G counts the distances twice, *i.e.*, $d(u,v)$ is included in $\Delta'(\mathrm{G},v;1)$ and in $\Delta'(\mathrm{G},u;1)$.

In this paper we examine the possibility of using the growth function to calculate the Wiener index of a helicene graph.

GROWTH IN [n]HELICENE GRAPHS

We will use the algorithm[11] for calculation of the growth function for graphs representing [n]helicenes. The idea of the algorithm is as follows: a graph is divided into subgraphs whose growth functions are then calculated recursively and included in the corresponding place to calculate the growth function of the whole graph.

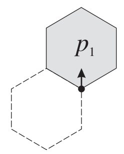
Let us limit ourselves to the case of vertex roots. The hexagon that includes the root is called a starting hexagon. Each hexagon adjacent to the starting hexagon is a derived hexagon and is used as the starting hexagon in the recursion process. For a root of the derived hexagon, we take the vertex that is the closest to the root of the starting hexagon. If there are two such vertices, both are denoted as a derived root, *i.e.*, we get an edge root. It can be seen that a derived root can only be a vertex root or an edge root. This observation is the key to the generalization presented in the next section.

When calculating the growth function of a graph by using the growth functions of its subgraphs the problem of counting some vertices twice must be avoided. The details of this procedure are discussed in the work of Lukšič and Pisanski.[11]

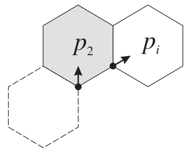
The [1]helicene is represented by only one hexagon, called a six cycle in graph theory[19] and denoted as C_6. Its growth is $\Delta(\mathrm{C}_6, r; x) = 1 + 2x + 2x^2 + x^3$ and is independent of the vertex r we take as the root. The case of [2]helicene is described in detail in Ref. 11 and thus left out.

We now consider the cases where the number of hexagons n is larger than 2. To find all possible growth functions of a graph H(n) representing an [n]helicene when the root is a single vertex, we have to calculate each of the growths separately depending on the root. This is done by determining which of the hexagon types defined in Lukšič and Pisanski[11] can occur in the case of [n]helicenes. Table II and Table III show the possible types of [n]helicenes depending of the root vertex. Let us use the notation from the mentioned work[11] for the labels p_1, p_2 and p_3 of the derived hexagons, which also correspond to the growth of the subgraphs they define (see Table I). The hexagons in gray in Table II and Table III denote the starting hexagons and the arrows show the path in which the growth is calculated recursively. This enables us to distinguish derived roots from the main root. The dashed hexagons show the possible continuation of the structure. A note about the symmetries is also needed since all of the types from Table I, Table II and Table III can be rotated and mirrored horizontally and vertically while still producing an identical growth function.

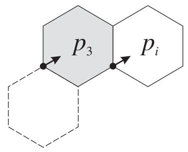
TABLE I. Possible derived hexagon types, labeled p_1, p_2 and p_3, in a graph representing an [*n*]helicene. Their labels are also used as the growth functions of the subgraphs starting with these (gray colored) hexagons. The dashed hexagons are from the previous step of recursion. Note that $i \in \{1,2\}$.



$p_1 = 1 + 2x + 2x^2 + x^3$



$p_2 = 1 + (1 + p_i)x + x^2 + x^3$



$p_3 = 1 + 2x + (1 + p_i)x^2$

The helical structure is even more useful when determining the possible derived hexagons. As seen from Table II and Table III, the derived hexagons can only be of types p_1, p_2 or p_3 as shown in Table I. If we encounter p_1, we know we are at one end of the chain. Besides type p_1, we can only get type p_2 as the derived hexagon after the second step of the recursion. Moreover, this is the only type we can get after the second step if we have a [$\pm\infty$]helicene.

Let us present an example of growth function calculation of a graph $H_1(n)$ representing an [*n*]helicene ($n > 2$) with the root vertex labeled 1 (see the first type in Table II). We write the system of equations that determine the growth of $H_1(n)$:

$$\Delta(H_1(n),1;x) = p_2^{(2)} + x + 2x^2 + x^3 ,$$

$$p_2^{(i)} = p_2^{(i+1)} x + 1 + x + x^2 + x^3 ,$$

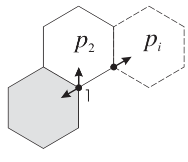
$$p_2^{(n)} = p_1 = 1 + 2x + 2x^2 + x^3 . \qquad (2)$$

The first equation in (2) is the growth function of $H_1(n)$ rooted at the vertex 1 (see Table II). The term $p_2^{(i)}$ represents the growth function of a subgraph of $H_1(n)$ that has its starting hexagon of type p_2 and the index i, where $1 < i < n$, denotes the i-th recursion step of the algorithm[11] calculating the growth. The last equation in (2) is the growth of the last hexagon in the chain forming a helicene. It can be shown that this system of equations forms the growth function of the graph $H_1(n)$ as

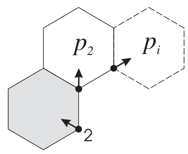
$$\Delta(H_1(n),1;x) =$$
$$1 + 3x + 5x^2 + 5x^3 + 4\sum_{i=4}^{n-1} x^i + 3x^n + x^{n+1}. \qquad (3)$$

However, the simplest proof of formula is by induction. Let us examine the change in the growth when a hexagon is added at the end of the structure, thus creating a [n+1]helicene. The growth function of a hexagon equals $1 + 2x + 2x^2 + x^3$ but since two of its vertices are shared with another hexagon, there are already included

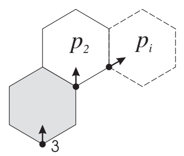
TABLE II. Possible helicene types with a vertex root when the starting hexagon (in gray) has only one neighbor ($i \in \{1,2\}$)



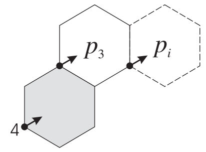
$\Delta(H,1; x) = p_2 + x + 2x^2 + x^3$



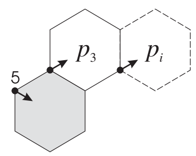
$\Delta(H,2; x) = 1 + (1 + p_2)x + x^2 + x^3$



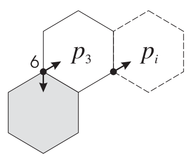
$\Delta(H,3; x) = 1 + 2x + (1 + p_2)x^2$



$\Delta(H,4; x) = 1 + 2x + (1 + p_3)x^2$

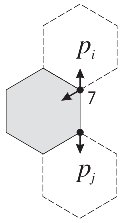
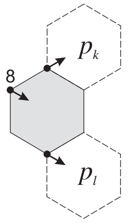
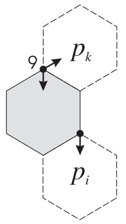


$\Delta(H,5; x) = 1 + (1 + p_3)x + x^2 + x^3$



$\Delta(H,6; x) = p_3 + x + 2x^2 + x^3$

TABLE III. Possible helicene types with a vertex root when the starting hexagon (in gray) has two neighbors ($i,j \in \{1,2\}$; $k,l \in \{1,3\}$)


$\Delta(\mathrm{H},7;x) = p_i + p_j x + x^2 + x^3$

$\Delta(\mathrm{H},8;x) = 1 + (1 + p_k)x + p_l x^2$

$\Delta(\mathrm{H},9;x) = p_k + x + (1 + p_i)x^2$

in the growth function of $\mathrm{H}_1(n)$. We therefore have to add only $x + 2x^2 + x^3$ to the growth function. Since the distance from the added hexagon to the root is $n - 1$, the expression gets multiplied by x^{n-1} yielding $x^n + 2x^{n+1} + x^{n+2}$. One can check that $\Delta(\mathrm{H}_1(n+1),1;x) - \Delta(\mathrm{H}_1(n),1;x)$ produces the same polynomial, thus proving formula (3).

If we rewrite formula (3) as

$$\Delta(\mathrm{H}_1(n),1;x) = -3 - x + x^2 + x^3 + 4\sum_{i=0}^{n-1} x^i + 3x^n + x^{n+1},$$

it holds for $n = 1$ and $n = 2$, too. Similar expressions are obtained if the vertex root is in a different position (see Table II). The exception is when there are two subgraphs derived from the starting hexagon as is the case in Table III. Then we must use another index that tells us how many hexagons are in one of such subgraphs.

The [7]helicene in Figure 1 is an another example of a helicene of the first type regarding to the types presented in Table II.

In order to get the Wiener index of a graph H(n) representing an [n]helicene, we must calculate the expression $\Delta'(\mathrm{H}(n),v;1)$ for each vertex $v \in \mathrm{H}$. We do this by using the growth function of a rooted graph $\mathrm{H}_v(n)$. For example,

$$\Delta'(\mathrm{H}_1(n),1;1) =$$

$$-1 + 2 + 3 + 4\sum_{i=0}^{n-1} i + 3n + n + 1 = 2n(n+1) + 5.$$

This procedure can be used to calculate the already known[8] Wiener index of an [n]helicene $W(\mathrm{H}(n)) = \frac{1}{3}(8n^3 + 72n^2 - 26n + 27)$.

We now extend the calculation of the growth function to the one-way infinite helicene graph $\mathrm{H}(\infty)$ rooted at r. We first select the root, *e.g.*, a vertex labeled 1, so that the rooted graph is $\mathrm{H}_1(\infty)$. Our system of equations consists only of the first two equations in (2). We can therefore write $p_2 = (1 + x + x^2 + x^3)/(1 - x)$ for $|x| < 1$. Hence,

$$\Delta(\mathrm{H}_1(\infty),1;x) =$$

$$\frac{1+x+x^2+x^3}{1-x} + x + 2x^2 + x^3 = \frac{(1+x)(1+x+x^2-x^3)}{1-x}.$$

The same argument holds with the other vertices as roots:

$$\Delta(\mathrm{H}_v(\infty),v;x) = \frac{f(x)}{1-x}, \qquad (4)$$

where v is the vertex root, $|x| < 1$ and $f(x)$ is a polynomial of a finite degree. Moreover, the formula (4) holds also for graphs representing two-way infinite helicenes.

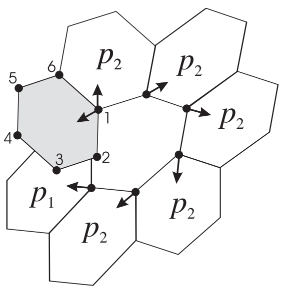


Figure 1. An example of a graph $\mathrm{H}_1(7)$ representing a [7]helicene rooted at the vertex 1. The labels p_1 and p_2 are used to identify the hexagon types for the growth calculation. The starting hexagon is colored gray with the labels showing the possible roots.

GROWTH IN FASCIAGRAPHS

In the previous section we noticed that only one of the hexagon types was repeating itself in the recursion process. The reason for this is in the way the growth calculation is transferred to the derived hexagons. Since two adjacent hexagons share a same edge, the growth function of that edge in the derived hexagon is always $1 + x$. If the starting root of the graph is an arbitrary connected subgraph, each derived hexagon has the growth on the adjacent edge either $1 + x$ or 2. This fact holds for all types of catacondensed polyhexes.[11]

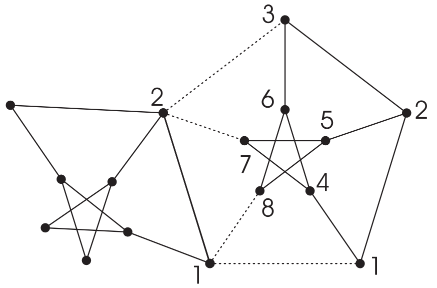


Figure 2. Fasciagraph γ_2(G;X), where G is a subgraph of the Petersen graphs and X = {{1,1},{3,2},{7,2},{8,1}}. The edges from X are dotted to separate them from the edges of G.

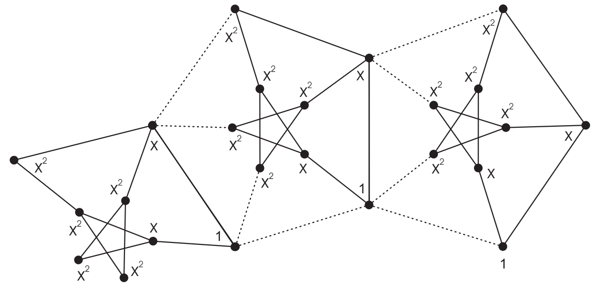


Figure 3. Fasciagraph γ_3(G,X) rooted at 1, where G and X are defined as in Figure 2. In each copy of the graph G the growth at its vertices is shown locally.

We can replace the hexagons representing benzene with an arbitrary connected graph and calculate the growth the same way as before. The new graph belongs to a subclass of fasciagraphs γ_m(G;X) that has its edges defined as $X \subseteq V(G) \times \{u,v\}$, where *u* and *v* are adjacent in G. An example can be seen in Figure 2 using a subgraph G of the well-known Petersen graph, labeling its vertices 1, 2,..., 8 and defining X = {{1,1},{3,2}, {7,2},{8,1}}. As a result we get a chain of $m-1$ Petersen graphs that ends with the graph G.

To calculate the growth functions of a fasciagraph γ_m(G;X) at its vertices we could use the same method as with the helicenes, *i.e.*, define the possible subgraph types γ_m(G;X) can be made up from, depending on what vertex we take for the root, and use them to calculate the growth recursively (the types for helicenes are seen in Table II and Table III). But, since G can be a large graph, there can be a lot of subgraph types. It is more interesting to find the growth at the adjacent vertices *u* and *v* that represent the ends of the edges from X. One or both of these vertices are in fact the root of the derived graphs (the generalization of derived hexagons). When looking at the growth at these vertices locally in the derived graph, it can be written as one of the following: $(1, x)$, $(x,1)$ or $(1,1)$, where the components represent the growth in *u* and *v*, respectively. Since the derived graphs are all the same, there must be a recurring pattern for the growth. From example in Figure 2 we can see how the growth at vertices 1 and 2 changes in the derived graph:

$$(1, x) \rightarrow (1, x),$$

$$(x,1) \rightarrow (1,1),$$

$$(1,1) \rightarrow (1, x).$$

Therefore, from some step onwards we always get a derived Petersen graph with the growth $(1, x)$ at vertices 1 and 2, respectively. That assures us that there is a compact form of writing the growth function. From example in Figure 3 we can deduce the growth function of the fasciagraph γ_3(G,X), where G and X are the same as in Figure 2 and the graph G is rooted in the vertex labeled 1. The growth equals $\Delta(\gamma_3(G;X),1; x) = 1 + 3x + 8x^2 + 7x^3 + 5x^4$ and can be easily generalized to

$$\Delta(\gamma_m(G;X),1; x) = -7 - 5x + 8\sum_{i=0}^{m-1} x^i + 7x^m + 5x^{m+1}$$

due to the recurring growth pattern $(1, x)$ for the vertices 1 and 2 in each of the derived graphs. If the graph would be one- or two-way infinite, we would get the same result as in the previous section; see formula (4). If G is an arbitrary connected graph, we can obtain similar conclusions by looking at the growth locally at the adjacent vertices *u* and *v*, where $X \subseteq V(G) \times \{u,v\}$.

CONCLUSIONS

In the paper we presented the concept of growth in rooted graphs. It was used on the simplest helicene graphs that represent [*n*]helicenes. The connection between the growth of a finite graph and its Wiener index was presented and used in the case of [*n*]helicenes. The growth calculation in both types of [*n*]helicenes (finite and infinite) was generalized to a subclass of fasciagraphs, where an arbitrary connected graph replaced the hexagonal rings. In further work, the growth function calculation is to be extended to all fasciagraphs as well as to the rotagraphs, which can be used to represent coronoids.

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SAŽETAK

Rast u $[n]$helicenima

Primož Lukšič i Tomaž Pisanski

Generirajuća funkcija za niz koji predstavlja broj čvorova grafa na danoj udaljenosti od korijena grafa zove se sferna funkcija rasta grafa s korijenom. Ova nova matematička veličina prvo je izračunata za konačne i beskonačne grafove koji predstavljaju $[n]$helicene a zatim je poopćena i izračunata za grafove u kojima je svaki heksagon zamijenjen proizvoljnim povezanim grafom te stoga predstavljaju podklasu tzv. fasciagrafova. Za konačne grafove uspostavljena je također veza između funkcije rasta i Wienerovog indeksa.