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HEXAGONAL SYSTEMS. A CHEMISTRY-MOTIVATED EXCURSION TO COMBINATORIAL GEOMETRY

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Abstract. Hexagonal systems are geometric objects obtained by arranging mutually congruent regular hexagons in the plane. Such geometric features are usually not considered in secondary-school courses of mathematics, although these are easy-to-grasp and probably interesting to students. In this paper the elements of the theory of hexagonal systems are outlined. We indicate some properties of hexagonal systems that secondary-school students could prove themselves, as well as a few less easy results and open problems.

ZDM Subject Classification: K34; *AMS Subject Classification*: 52C20, 97A20.

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1. Introduction

In this article we intend to make the reader (assumed to be a mathematics teacher or secondary-school student interested in mathematics or university student of mathematics) familiar with hexagonal systems and their theory. Before any formal definition, it is purposeful to show a few examples. These are found in Fig. 1. In fact in Fig. 1 are displayed all (mutually distinct) hexagonal systems with 2, 3, and 4 hexagons.

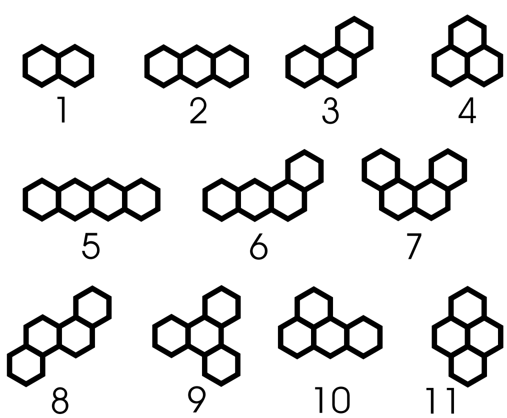

Fig. 1. All hexagonal systems with $h = 2, 3, 4$ hexagons.

Most readers will immediately understand what we are speaking about. This would especially apply to secondary-school students who may and should skip the somewhat boring definitions that follow.

For some readers it may be stimulating to know that in chemistry there exists a class of so-called *benzenoid hydrocarbons* whose structures fully coincide with those of hexagonal systems. In Fig. 2 we show the chemical formula of a compound called benzo[*a*]pyrene and the corresponding hexagonal system. In this article we will not go into any further chemical detail (which can be found in the books [1,2]), but only mention that the properties of hexagonal systems were, and currently still are, much studied just because of their chemical relevance.

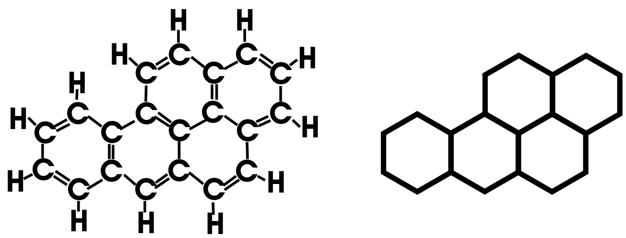

Fig. 2. The structural formula of a benzenoid hydrocarbon called benzo[*a*]pyrene and the corresponding hexagonal system; the coincidence should be self-evident. Note that benzo[*a*]pyrene is one of the constituents of tobacco smoke, causing various forms of cancer to those who are inhaling tobacco smoke.

It is known that the plane can be covered (tiled) by only three regular polygons: regular triangles, squares and regular hexagons.

Exercise 1. Check the above statement.

The plane covered by regular hexagons is called the *hexagonal lattice*, see Fig. 3. The hexagonal lattice consists of lines, that in what follows will be called *edges*, and points in which three lines meet, that in what follows will be called *vertices*. Every edge connects two vertices which are said to be its endpoints.

Definition 1. Let $v_1, v_2, v_3, \ldots, v_k$ be k mutually distinct vertices of the hexagonal lattice. A *cycle* on the hexagonal lattice is an ordered k-tuple of edges $[e_1, e_2, \ldots, e_{k-1}, e_k]$, such that the endpoints of the edge e_1 are the vertices v_1 and v_2, the endpoints of the edge e_2 are the vertices v_2 and v_3, $\ldots$, the endpoints of the edge e_{k-1} are the vertices v_{k-1} and v_k, and the endpoints of the edge e_k are the vertices v_k and v_1. The size of this cycle is k.

Definition 2. Let C be a cycle on the hexagonal lattice. Then the collection of vertices and edges of the hexagonal lattice that lie on C and in the interior of C form a *hexagonal system*. Any hexagonal system is determined by means of some cycle on the hexagonal lattice. The cycle C is said to be the *boundary* of the respective hexagonal system.

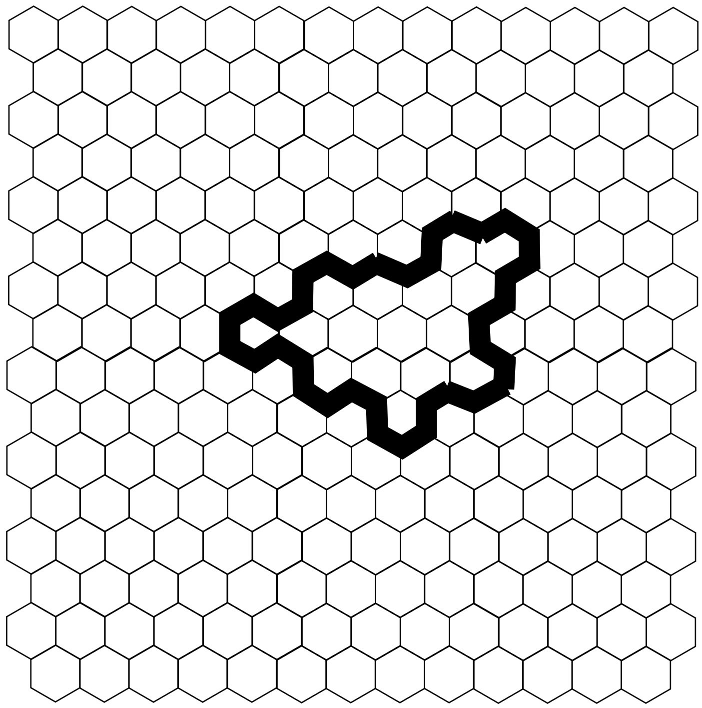

Fig. 3. The hexagonal lattice and a cycle C on it. This cycle forms the boundary of a hexagonal system. The hexagonal system determined by means of C is shown in Fig. 4.

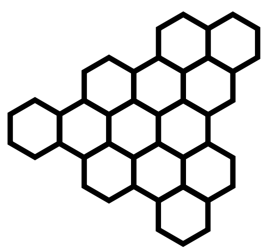

Fig. 4. The hexagonal system determined by the cycle C from Fig. 3.

An example illustrating Definition 2 is found in Figs. 3 and 4.

Without loss of generality, the edges of both the hexagonal lattice and of all hexagonal systems will be drawn so that some of them are vertical. Further, the edges of all hexagonal systems will be assumed to be of equal length, say of unit length.

The number of hexagons of a hexagonal system will be denoted by h.

From Definition 2 we see that a hexagonal system is a planar geometric object consisting of several (h) mutually congruent regular hexagons. Two such hexagons are either disjoint (i.e., have no vertex or edge in common) or share exactly one edge and (therefore) exactly two vertices. The hexagonal system divides the plane into one infinite domain and h finite domains, each of which are regular hexagons.

DEFINITION 3. Two hexagonal systems A and B are considered to be congruent (that is: identical) if B can be brought into coincidence with A by means of translation and/or rotation and/or reflection.

In Fig. 5 are shown the mutually equivalent ways in which a hexagonal system can be drawn. Assuming that some edges are vertical, there are at most twelve such representations (as shown in Fig. 5).

EXERCISE 2. Why twelve?

If the hexagonal system is symmetric, then the number of its equivalent representations is less than twelve.

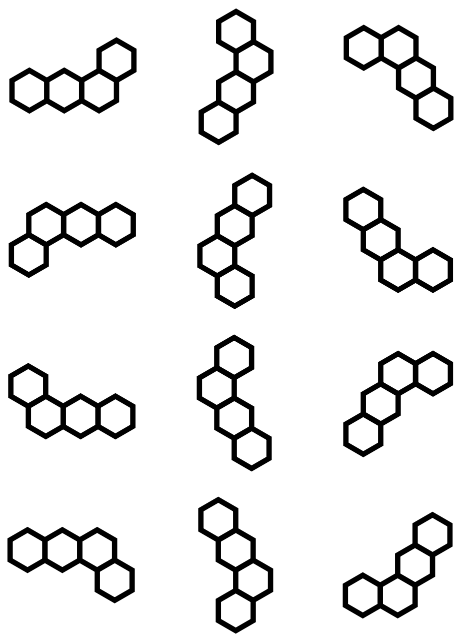

Fig. 5. The twelve different ways in which the hexagonal system **6** from Fig. 1 can be drawn, assuming that some of its edges are vertical.

EXERCISE 3. Show that the hexagonal systems **4** and **11** have two and three equivalent representations, respectively. Construct a hexagonal system whose representation is unique.

2. How many hexagonal systems?

Already from Fig. 1 we see that for $h \geq 3$ there are more than one hexagonal systems with h hexagons. Therefore the natural question is: how many? This turned out to be a very difficult question.

Denote by H_h the number of hexagonal systems with h hexagons. Of course, we are interested only in mutually non-congruent species, in the sense of Definition 3.

From Fig. 1 we see that $H_2 = 1$, $H_3 = 3$, $H_4 = 7$. It is immediately realized that $H_1 = 1$.

Exercise 4. Show that $H_5 = 22$ by constructing all hexagonal systems with 5 hexagons. For beginners this may be difficult and error-prone. An ambitious reader may try to do the same for H_6, but nobody is advised to go beyond $h = 6$.

In fact, the number of hexagonal systems with h hexagons rapidly increases with h. For instance:

h	H_h
5	22
6	81
7	331
8	1 435
9	6 505
10	30 086
15	74 207 910
20	205 714 411 986
25	606 269 126 076 178
30	1 857 997 219 686 165 624
35	5 851 000 265 625 801 806 530

At the present moment the number of hexagonal systems for $h > 35$ is not known. All the hitherto determined H_h-values were obtained by computer-aided counting. The mathematical solution of this problem was attempted long time ago [3], but so far without any success. Because many other similar enumerations in combinatorics could be relatively easily achieved [3], the American mathematician Frank Harary (1921–2005) offered in 1968 an award of US$ 100 for solving the problem. Until now nobody claimed the prize.

It is unlikely that one can find an expression showing how H_h depends on h. However, it would be of great value to establish the asymptotic behavior of H_h for $h \to \infty$. This also is not known.

Based on the available values of H_h (up to $h = 35$) it was estimated [4] that the asymptote has the form

$$H_h \sim \frac{\alpha\, h^{\beta}}{\gamma^{h}}$$

where α, β, and γ are some constants. Whereas $\alpha \approx 0.0234$ and $\beta \approx 5.1619$ are evidently not simple numbers, numerical calculations (based on the data for $h \leq 35$) show that $\gamma = 1.00000 \pm 0.00001$. It seems very likely that γ is exactly equal to unity, but nobody knows how to prove this fact.

In summary: At the present moment the answer to the question posed in the title of this section is: *We don't know.*

3. On the Anatomy of Hexagonal Systems

Until now we have learned that hexagonal systems contain *vertices, edges*, and *hexagons*. The number of these structural features will be denoted by n (= number of vertices), m (= number of edges), and h (number of hexagons). In what follows we will prove that these three parameters are related as

$$m = n + h - 1\ . \tag{1}$$

From Definition 2 we know what the *boundary* of a hexagonal system is. The vertices lying on the boundary are said to be *external.* The vertices lying inside the boundary (if any) are said to be *internal.* The number of internal vertices will be denoted by n_i. Then we have,

Theorem 1. *For any hexagonal system with n vertices, m edges, h hexagons, and n_i internal vertices,*

$$n = 4h + 2 - n_i \tag{2}$$

$$m = 5h + 1 - n_i\ . \tag{3}$$

Proof. We will prove Eqs. (2) and (3) by mathematical induction on the number h of hexagons. In order to do this we have to perform three steps.

1. The validity of both Eqs. (2) and (3) can be directly checked for the unique hexagonal system with $h = 2$ (**1** in Fig. 1) and for the three hexagonal systems with $h = 3$ (**2**, **3**, and **4** in Fig. 1).

For example, the hexagonal system **4** has $n = 13$ vertices, $m = 15$ edges, and a single internal vertex, $n_i = 1$. Indeed, $13 = 4 \cdot 3 + 2 - 1$ and $15 = 5 \cdot 3 + 1 - 1$. We leave to the reader the examination of the hexagonal systems **1**, **2**, and **3**, as well as of the case $h = 1$.

2. Assume now that Eqs. (2) and (3) hold for all hexagonal systems with less than h hexagons, in particular for hexagonal systems with $h - 1$ hexagons. Let X be a hexagonal system with $h - 1$ hexagons, with $n(X)$ vertices, $m(X)$ edges and $n_i(X)$ internal vertices. Assume thus that the equalities

$$n(X) = 4(h-1) + 2 - n_i(X) \quad \text{and} \quad m(X) = 5(h-1) + 1 - n_i(X)$$

are satisfied. These are just special cases of Eqs. (2) and (3). For our needs these equalities will be rewritten as

$$n(X) - 4(h-1) - 2 + n_i(X) = 0 \tag{4}$$

$$m(X) - 5(h-1) - 1 + n_i(X) = 0 \ . \tag{5}$$

3. Let Y be a hexagonal system obtained by adding to X a new hexagon. Then, of course, Y has h hexagons. Adding a new hexagon to X can be done in five different ways, as shown in Fig. 6. Therefore we need to separately consider five cases.

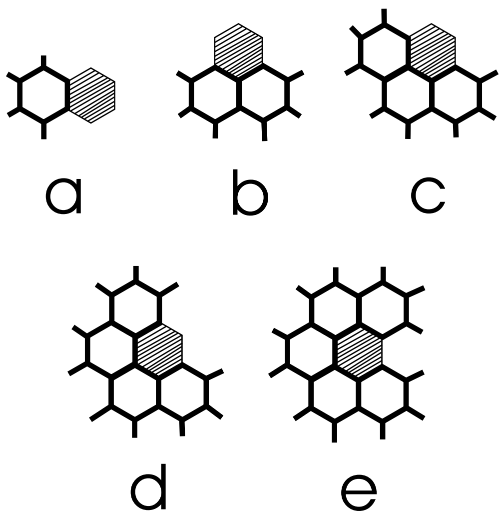

Fig. 6. The five ways in which a new hexagon (indicated by hatching) can be added to a hexagonal system.

Case a. By adding a new hexagon to X in mode **a**, as shown in Fig. 6, the number of vertices is increased by 4, the number of edges is increased by 5, and the number of internal vertices remains unchanged. Hence, $n(X) = n(Y) - 4$, $m(X) = m(Y) - 5$, $n_i(X) = n_i(Y)$. Substituting these relations back into (4) and (5) we obtain

$$n(Y) - 4 - 4(h-1) - 2 + n_i(Y) = 0$$
$$m(Y) - 5 - 5(h-1) - 1 + n_i(Y) = 0$$

i.e.,

$$n(Y) = 4h + 2 - n_i(Y) \tag{6}$$

$$m(Y) = 5h + 1 - n_i(Y) \tag{7}$$

i.e., relations (2) and (3) are satisfied in Case a.

Case b. By adding a new hexagon to X in mode **b**, as shown in Fig. 6, the number of vertices is increased by 3, the number of edges is increased by 4, and the number of internal vertices is increased by 1. Hence, $n(X) = n(Y) - 3$, $m(X) = m(Y) - 4$, $n_i(X) = n_i(Y) - 1$. Substituting these relations back into (4) and (5) we obtain

$$n(Y) - 3 - 4(h-1) - 2 + n_i(Y) - 1 = 0$$
$$m(Y) - 4 - 5(h-1) - 1 + n_i(Y) - 1 = 0$$

which again lead to Eqs. (6) and (7), implying that the relations (2) and (3) are satisfied also in Case b.

Cases c, d, and e are treated in a fully analogous manner. We leave this part of the proof to the reader.

After examining all the five cases, we verify that if the relations (2) and (3) are obeyed by a hexagonal system X with $h-1$ hexagons, then they are obeyed also by the hexagonal system Y with h hexagons.

Any hexagonal system with h hexagons can be obtained by adding a hexagon to some hexagonal system with $h-1$ hexagons. Bearing this in mind we conclude that if the relations (2) and (3) are obeyed by the hexagonal systems with $h-1$ hexagons, then they are obeyed also by the hexagonal systems with h hexagons. In the step 1 of our proof we showed that the relations (2) and (3) are obeyed in the case $h = 3$. Therefore these are obeyed also in the case $h = 4$, and therefore also in the case $h = 5$, and therefore also in the case $h = 6$, etc. Therefore Eqs. (2) and (3) are obeyed for any value of h.

By this the proof of Theorem 1 is completed. ■

By subtracting Eq. (3) from Eq. (2), thus eliminating from them n_i, we arrive at:

Theorem 2. *Eq. (1) holds for any hexagonal system with n vertices, m edges, and h hexagons.*

Hexagonal systems possess a large number of cycles. For instance, the hexagonal system **4**, depicted in Fig. 1, has a total of 7 cycles, shown in Fig. 7.

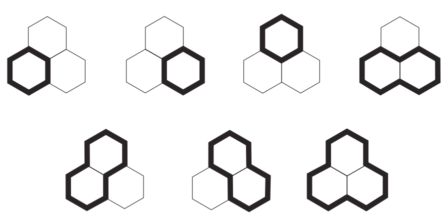

Fig. 7. The seven cycles (indicated by heavy lines) contained in the hexagonal system **4** from Fig. 1. Three cycles are of size 6, three of size 10, and one of size 12.

EXERCISE 5. Check that the hexagonal systems **1**, **2**, and **3** from Fig. 1 possess 3, 6, and 6 cycles, respectively. Note that counting the cycles in larger hexagonal systems, e.g., in the one depicted in Fig. 4, is a hopelessly difficult task.

It is easy to see that the cycles contained in hexagonal systems may be of size 6, 10, 12, 14, 16, … . In other words, the size of a cycle contained in a hexagonal system may be any positive even number, except 2, 4, and 8.

The following result plays an important role in the theory of hexagonal systems [5]. Let C be a cycle of a benzenoid system and $|C|$ its size.

THEOREM 3. *Let C is a cycle of a hexagonal system. If $|C|$ is divisible by 4, then in the interior of C there is an odd number of vertices. If $|C|$ is not divisible by 4, then in the interior of C there are either no vertices, or their number is even.*

Proof. In the sense of Definition 2, the cycle C may be viewed as the boundary of some hexagonal system. If so, then this hexagonal system possesses $n = |C| + n_i$ vertices, where n_i is just the number of vertices in the interior of C. Using Eq. (2) we get

$$|C| + n_i = 4h + 2 - n_i$$

from which follows

$$n_i = 2h + 1 - \frac{1}{2}\,|C| \ . \tag{8}$$

Now, if $|C|$ is divisible by 4, then $\frac{1}{2}\,|C|$ is even, and then the right-hand side of (8) is odd. Otherwise, if $|C|$ is even, but not divisible by 4, then the right-hand side of (8) is even.

This proves Theorem 3. ■

The hexagonal systems that do not possess internal vertices, $n_i = 0$, are said to be *catacondensed*. If $n_i > 0$ then one speaks of *pericondensed* hexagonal systems. In Fig. 1 the hexagonal systems **1**, **2**, **3**, **5**, **6**, **7**, **8**, and **9** are catacondensed whereas **4**, **10**, and **11** are pericondensed.

Theorem 3 has a noteworthy consequence: The size of any cycle of a catacondensed hexagonal system is even, but not divisible by 4. Thus catacondensed hexagonal systems possess only cycles of size 6, 10, 14, 18, … .

EXERCISE 6. Show that every pericondensed hexagonal system possesses a cycle of size 12.

A vertex of a hexagonal system is incident to either two edges or to three edges. In the theory of hexagonal systems one says that a vertex is either of *degree* two (if it is the endpoint of two edges) or of degree three (if it is the endpoint of three edges). The number of vertices of degree 2 and 3 will be denoted by n_2 and n_3, respectively. Note that $n_2 + n_3 = n$.

For instance, the hexagonal system **4** from Fig. 1 has $n_2 = 9$ and $n_3 = 4$.

THEOREM 4. *A hexagonal system with h hexagons has $2(h-1)$ vertices of degree 3, i.e., $n_3 = 2h - 2$.*

Proof. Observe first that for the hexagonal systems with $h = 1$ and $h = 2$ it is $n_3 = 0$ and $n_3 = 2$, in agreement with Theorem 4. Consider now the addition of a new hexagon, as shown in Fig. 6. It is easily verified that in whichever way we add the new hexagon, the number of vertices of degree 3 will increase by two. Theorem 4 follows. ■

EXERCISE 7. Show that $n_2 = 2h + 4 - n_i$.

We end this article by stating without proof a beautiful result by Harary and Harborth [6], determining the intervals in which the parameters n, m, and h can vary. Let $\lceil x \rceil$ denote the smallest integer that is greater than or equal to x. For example, $\lceil 2.8 \rceil = 3$, $\lceil 3.0 \rceil = 3$, $\lceil 3.2 \rceil = 4$, $\lceil \pi \rceil = 4$.

THEOREM 5. *For a hexagonal system with* n *vertices,* m *edges, and* h *hexagons,*

$$2h + 1 + \left\lceil \sqrt{12\,h - 3} \right\rceil \;\leq\; n \;\leq\; 4h + 2$$

$$3h + \left\lceil \sqrt{12\,h - 3} \right\rceil \;\leq\; m \;\leq\; 5h + 1$$

$$\left\lceil \frac{n-2}{4} \right\rceil \;\leq\; h \;\leq\; n + 1 - \left\lceil \frac{n + \sqrt{6n}}{2} \right\rceil$$

$$n - 1 + \left\lceil \frac{n-2}{4} \right\rceil \;\leq\; m \;\leq\; 2n - \left\lceil \frac{n + \sqrt{6n}}{2} \right\rceil$$

$$\left\lceil \frac{m-1}{5} \right\rceil \;\leq\; h \;\leq\; m - \left\lceil \frac{2m - 2 + \sqrt{4m+1}}{3} \right\rceil$$

$$1 + \left\lceil \frac{2m - 2 + \sqrt{4m+1}}{3} \right\rceil \;\leq\; n \;\leq\; m + 1 - \left\lceil \frac{m-1}{5} \right\rceil \;.$$

These bounds are the best possible: any combination of n, m, *and* h *satisfying the above inequalities may occur. In particular, hexagonal systems exist for all* n, *except* $n < 6$ *and* $n = 7, 8, 9, 11, 12, 15$, *and for all* m, *except* $m < 6$ *and* $m = 7, 8, 9, 10, 12, 13, 14, 17, 18, 22$.

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