UNIVERZITET U NOVOM SADU
PRIRODNO-MATEMATIČKI FAKULTET
DEPARTMAN ZA MATEMATIKU I INFORMATIKU

Multidisciplinarnost u istraživanju – pojam i jedna studija slučaja

Dr Dragan Mašulović

ERASMUS+ PROJECT
Re@WBC
Enhancement of HE research potential contributing to further growth of the WB region

Šta je to multidisciplinarnost?

- Znanje iz jedne discipline ponekad nije dovoljno za rešenje nekog naučnog ili stručnog zadatka
- Multidisciplinarna istraživanja okupljaju istraživače iz više različitih disciplina kako bi se rešili naučno-istraživački zadaci iz specifične oblasti

Širi kontekst

- **Intradisciplinarnost** (koncentracija) se odnosi na istraživanje u jednoj oblasti
- **Multidisciplinarnost** (aditivnost) se zasniva na znanju iz različitih disciplina ali ostaje unutar njihovih granica. Istraživači iz različitih disciplina rade na istom istraživačkom zadatku, ali svako svoj rad zasniva na znanju iz svoje discipline
- **Interdisciplinarnost** (integracija) analizira, integriše i harmonizuje znanje iz više disciplina u koherentnu celinu. Discipline se mestimično preklapaju.
- **Transdiciplinarnost** (holističnost) integriše znanje iz različitih disciplina ali se prostire i van njih.
- **Krosdisciplinarnost** se odnosi na posmatranje jedne discipline iz perspektive druge discipline

Prilike

- Bolje razumevanje problema uz pogled iz drugačije perspektive
- Nemoguće postaje moguće
- Primena inovativnih metoda u rešavanju problema
- Veći impakt istraživanja
- Brže rešavanje problema – efikasnost istraživanja
- Stvaranje efikasnijih rešenja

Pretnje

- **Istraživačka komunikacija**
  - Svaka disciplina koristi svoje definicije, terminologiju i žargon
  - Članovi timova koriste različita značenja za isti pojam (model mandibule)
  - Članovi timova ne razumeju značenje pojedinih pojmova (graft)
  - Sujeta – ne prihvatanje dobrih predloga drugih istraživača
  - Ljudi nerado priznaju da im nešto nije jasno
  - Mišljenje da su sastanci interdisciplinarnih timova gubljenje vremena

Pretnje

- **Poslovna komunikacija**
  - Redovnost u odgovaranju na mejlove
  - Formalnosti u komunikaciji
  - Nepotpune informacije
  - Korišćenje kolaboracionih portala
  - Frekvencija organizacije sastanaka
  - Jezičke barijere
  - Kulturološke barijetre (komunikacija samo sa istim polom)
  - Običaji u komunikaciji (komunikacija samo sa kolegama na istom nivou)

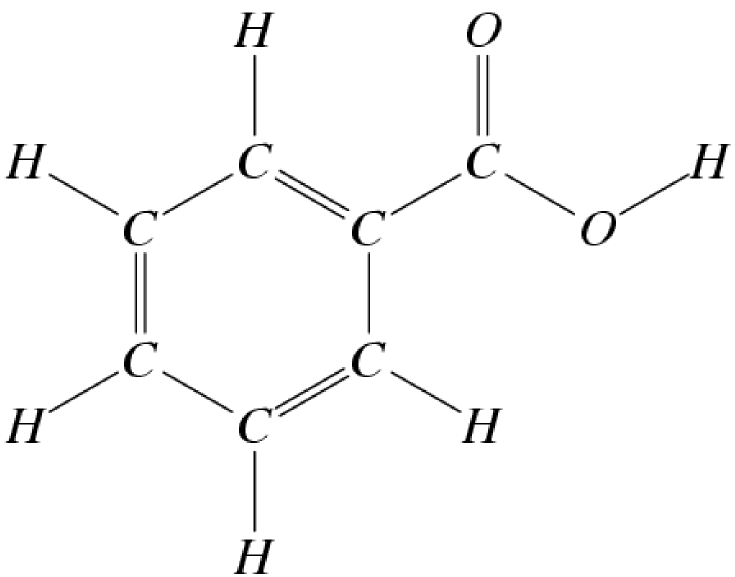
Pretnje

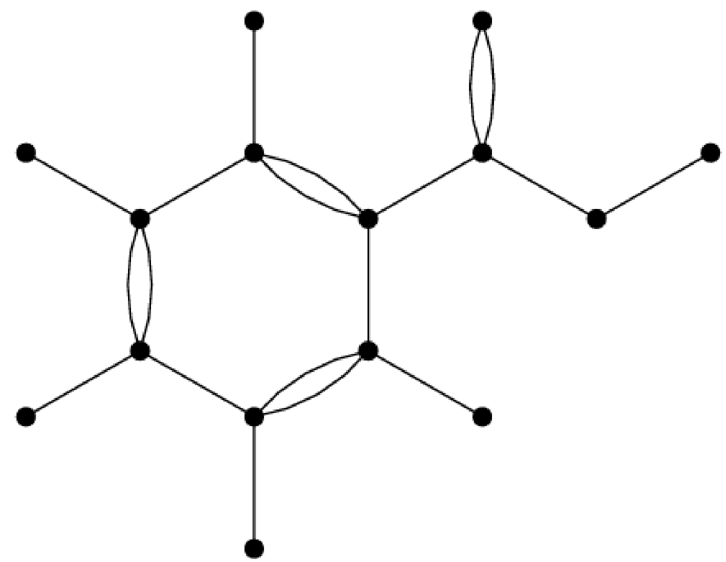
- **Stil rada**
  - Samostalni i timski rad
  - Plan i protokol istraživanja
  - Poštovanje rokova
  - Svest o etičkoj dimenziji istraživanja
  - Publikovanje rezultata
  - Diseminacija informacija o projektu
  - Komercijalizacija rezultata
  - Poštovanje institucionalne hijerarhije

Pretnje

- **Integritet istraživanja**
  - Kvantitativni ili kvalitativni rezultati
  - Nmeričke simulacije ili eksperiment
  - Protokol eksperimenata
  - Citiranje
  - Važeće norme u disciplini

STUDIJA SLUČAJA: MODELIRANJE U HEMIJI





```
begin
    initialize Cage(h);
    set total[1 ... h] to 0;
    for q := 0 to h − 1 do
        initialize y-axis key hexagon(q);
        ExpandLeftPart(LeftInitPos(q), InitBdrHexgns(q))
    od
end
```

Motivation

- If we wished to synthesize a new chemical compound with more desirable properties in comparison to the compounds already known, the standard procedure would be to identify and test candidate compounds.

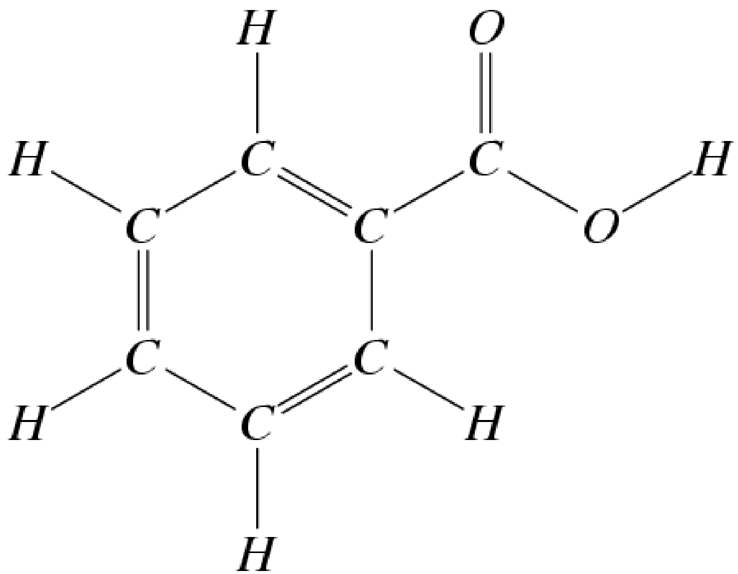
- Such experimental tests are very expensive and time consuming.

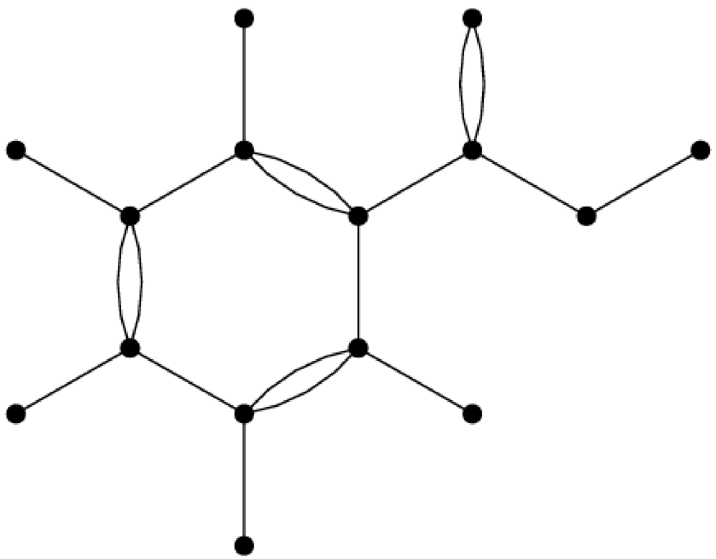
Motivation

- We can instead produce a **combinatorial library** consisting of structural formulas of candidate compounds and analyze **virtual** compounds by means of fast algorithms.
- This inexpensive approach can scan a much greater range of candidate compounds and thus reduce the vast number of possibilities to a practically feasible few, which can then be tested using standard procedures.

Graphs as models of structures

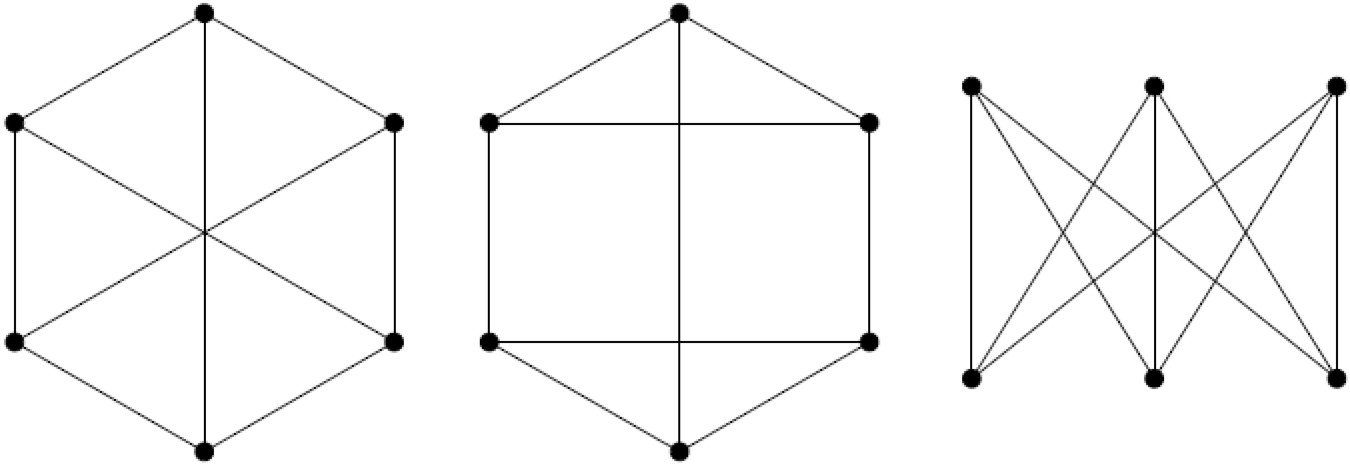
- Graphs represent one of the most popular tools for modeling discrete phenomena where the abstraction of the problem involves information about certain objects being connected or not
- The structural formula of benzoic acid $C_7H_6O_2$:





Graphs as models of structures

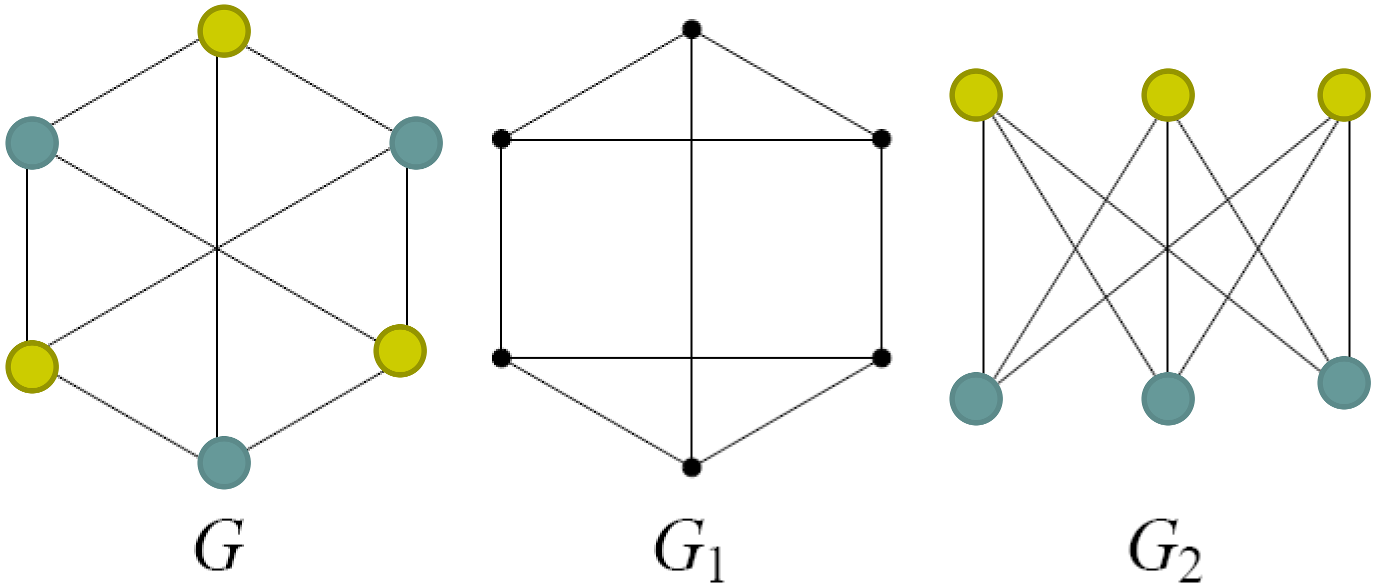
- isomorphism of graphs



G G_1 G_2

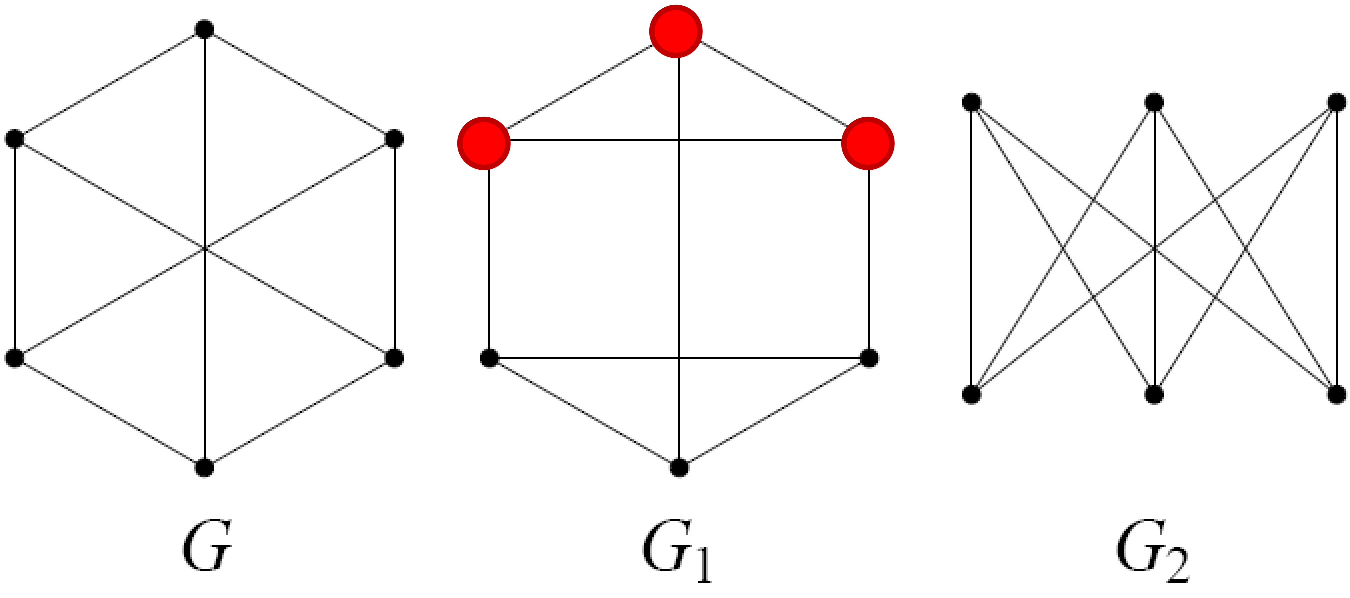
Graphs as models of structures

- isomorphism of graphs



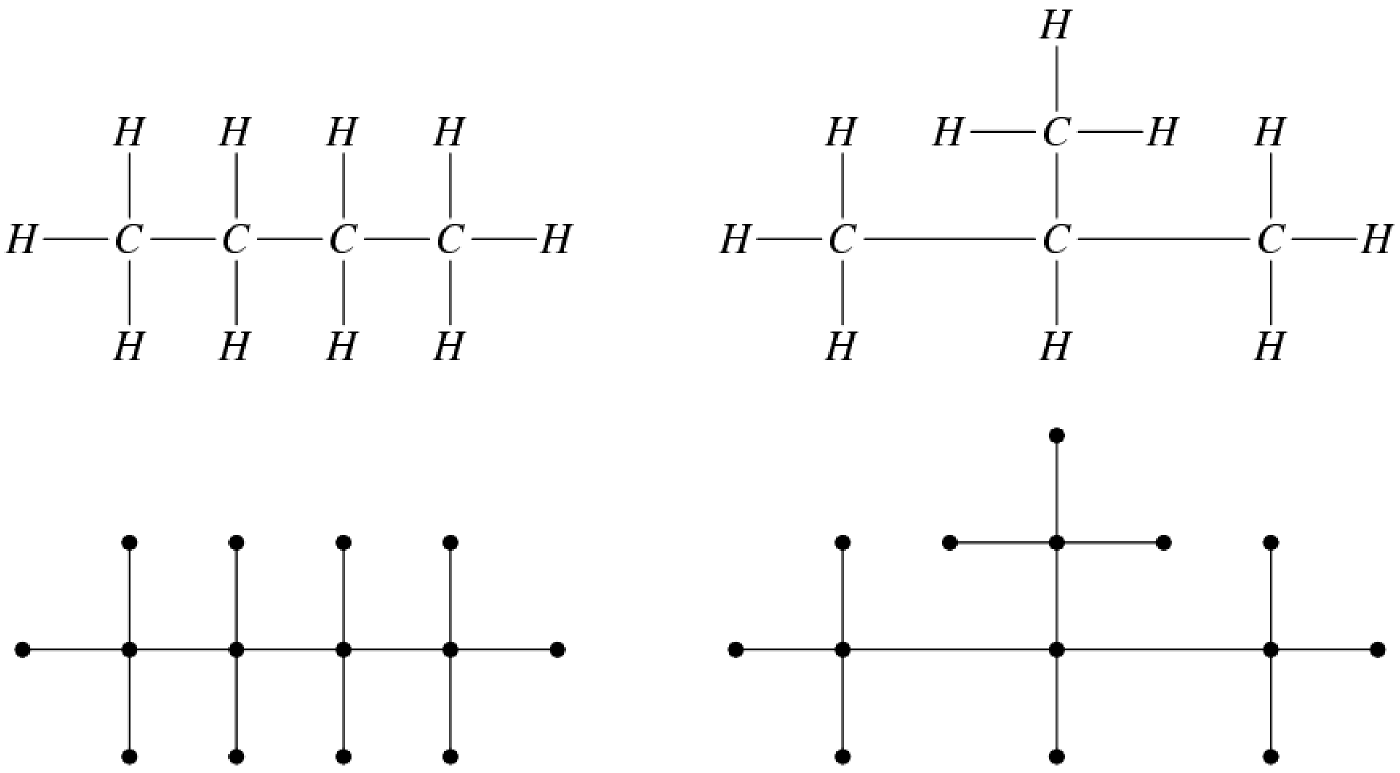
Graphs as models of structures

- isomorphism of graphs



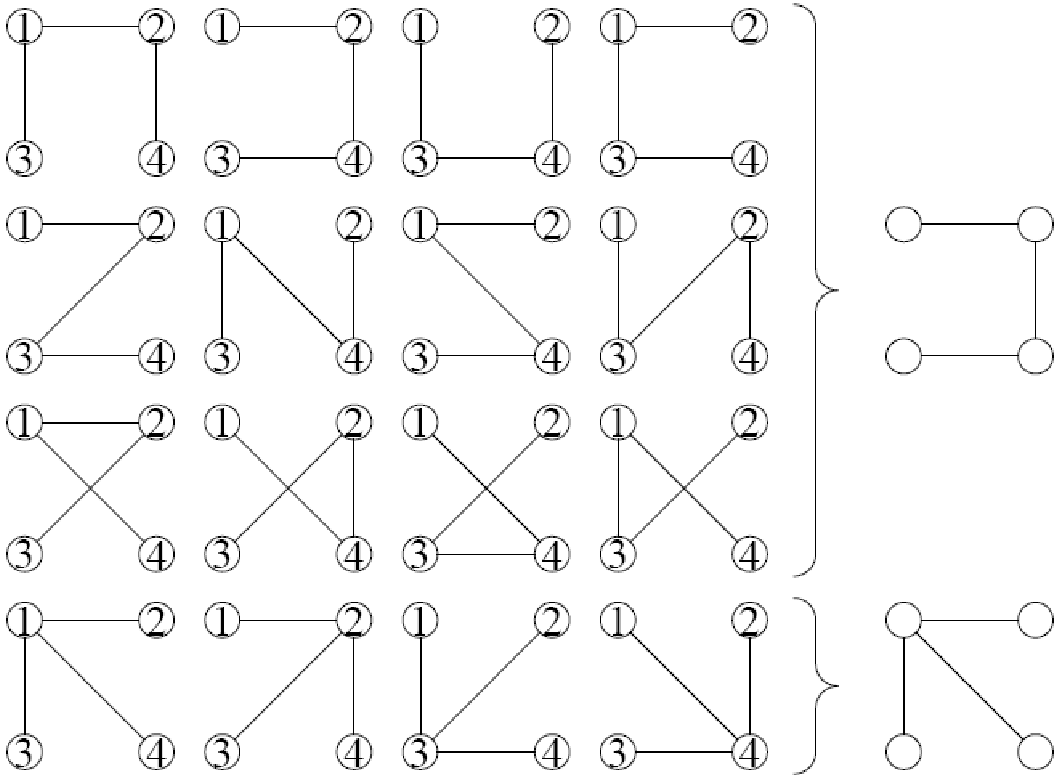
Trees

- A. Cayley (1889): counting isomers of carbohydrates



Trees

- Counting distinct structures VS Counting nonisomorphic structures



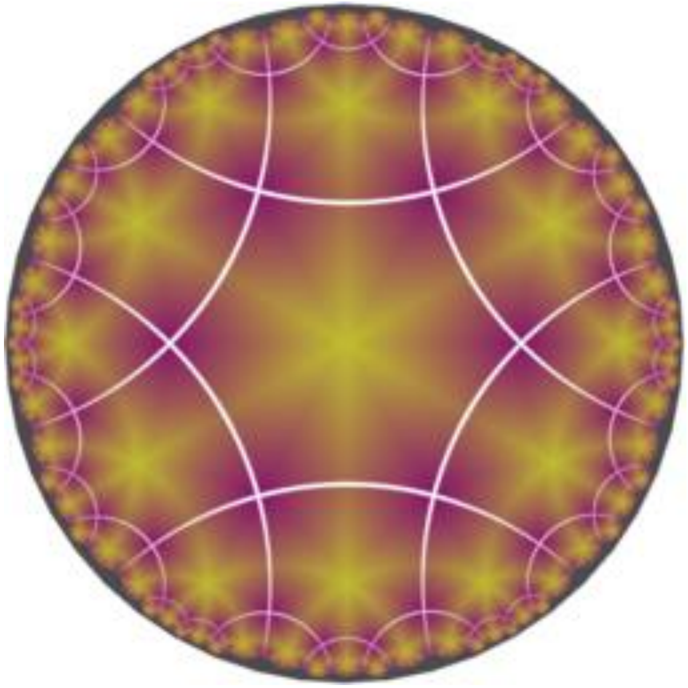
Trees

- **Cayley's Theorem.**
  There are n^{n-2} ***distinct*** *trees on n vertices.*

- But how many nonisomorphic (essentially distinct) ones?

Advanced topic: Structure and Symmetry

- Symmetry ←→ Automorphism
- Example: hexagon
  - axial symmetries & rotations
  - D6
- Symmetric structures are rich in automorphisms



Advanced topic: Structure and Symmetry

- Permutation group
- Aut(S) – the group of automorphisms of S
- If S is highly symmetric, |Aut(S)| is large
- Example:
  - K_n
  - S_n
  - C_n
  - P_n

Advanced topic: Structure and Symmetry

- Groups acting on sets
- Orbits of a group action
- **Cauchy-Frobenius (Burnside) Lemma**

$$|X/G| = \frac{1}{|G|} \sum_{g \in G} |\mathrm{fix}(g)|$$

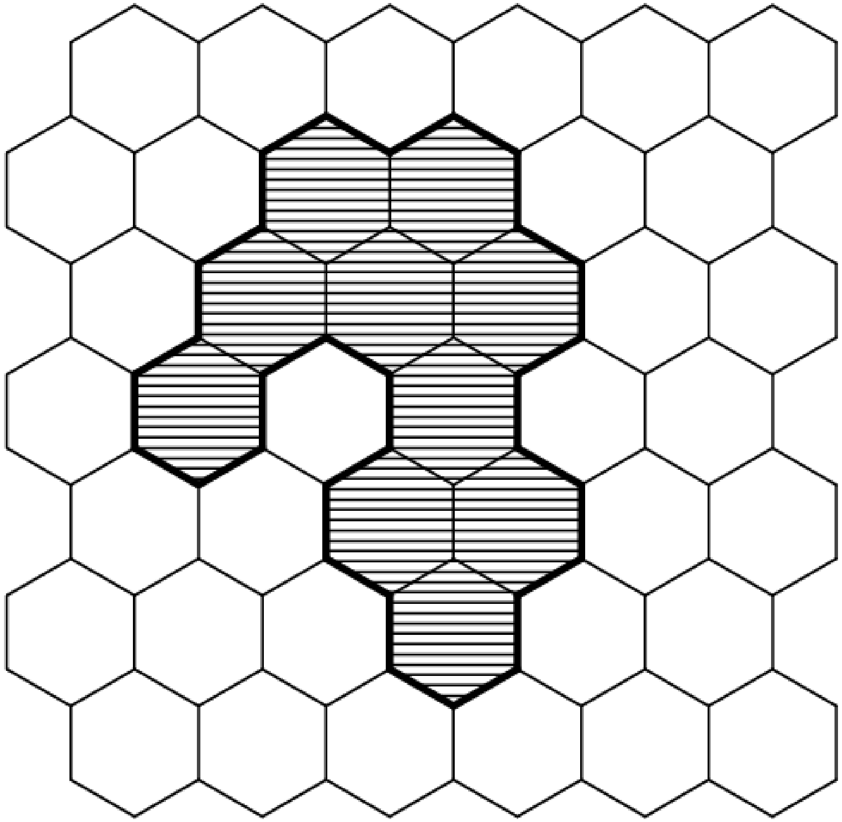
Advanced topic: Counting hexagonal systems

- A classical paper on counting polyhex hydrocarbons dates back to 1968:

  Balaban, Harary: *Chemical Graphs, Enumeration and Proposed Nomenclature of Benzenoid Cata-Condensed Polycyclic Aromatic Hydrocarbons,* Tetrahedron 24 (1968), 2505—2516

Advanced topic: Counting hexagonal systems

- A planar simply connected hexa-gonal system (HS):
- Find the number of non-isomorphic HS's with *h* hexagons



Advanced topic: Counting hexagonal systems

- There is no general formula for the number of nonisomorphic hexagonal systems!

- enumeration using brute force:
fast computers and algorithms

- In 1983 the Düsseldorf-Zagreb group (Knop and Trinajstić with collaborators) published their results from computerized enumerations hexagonal systems to $h = 10$

Advanced topic: Counting hexagonal systems

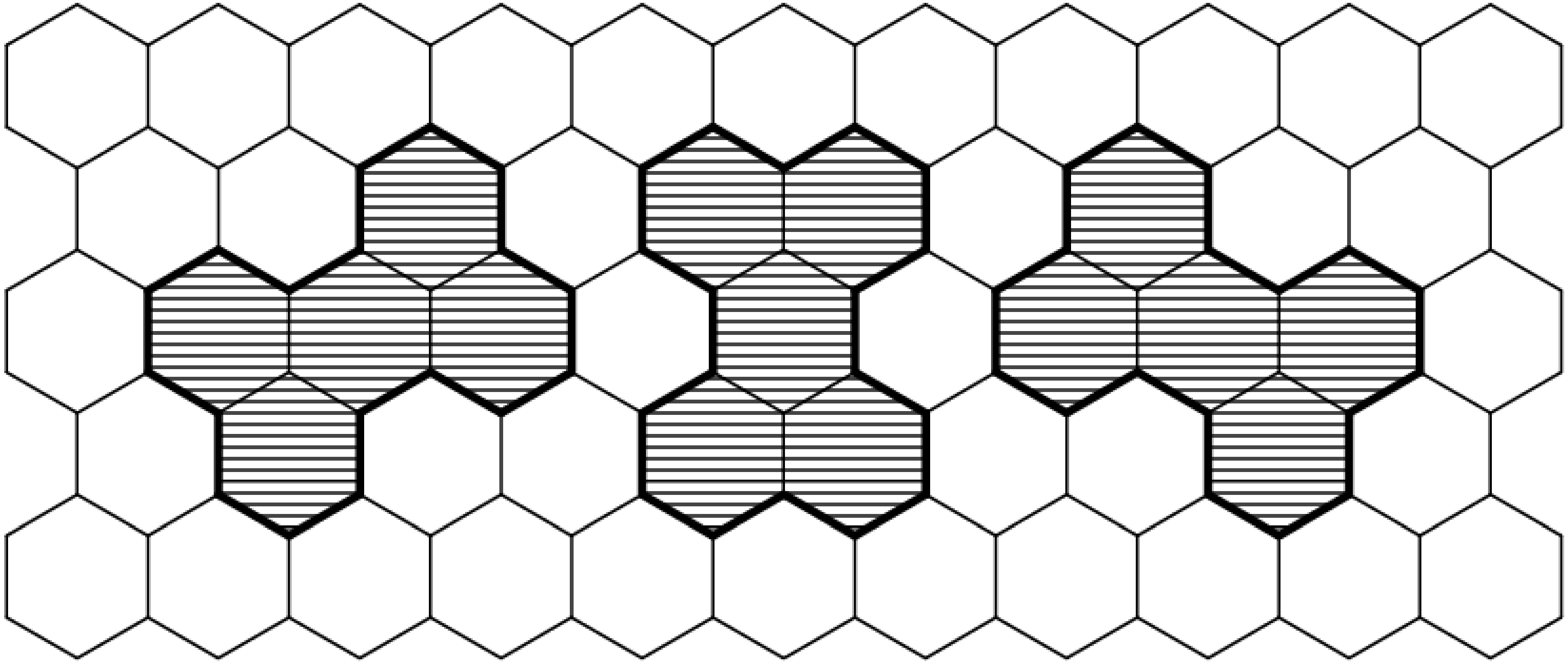
- What we are going to show is just the main idea of the algorithm presented in

  Tošić R., Mašulović D., Stojmenović I., Brunvoll J., Cyvin B. N., Cyvin S. J., *Enumeration of Polyhex Hydrocarbons to h = 17*, J. Chem. Inf. Comput. Sci., 35(2) (1995) 181-187

- Many purely technical details had to be added in order to make a working computer program out of it.

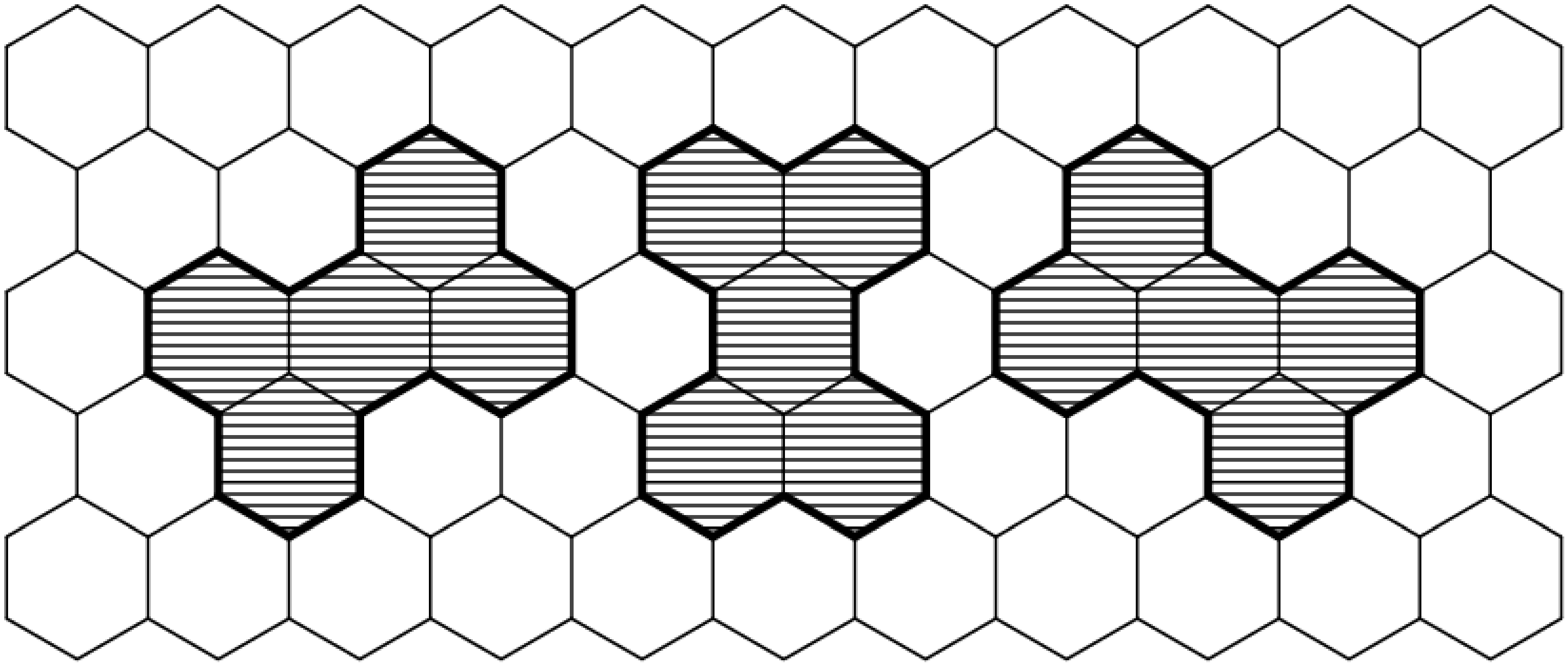
Advanced topic: Counting hexagonal systems

- Hexagonal systems are *isomorphic* if they are congruent in the sense of euclidean geometry



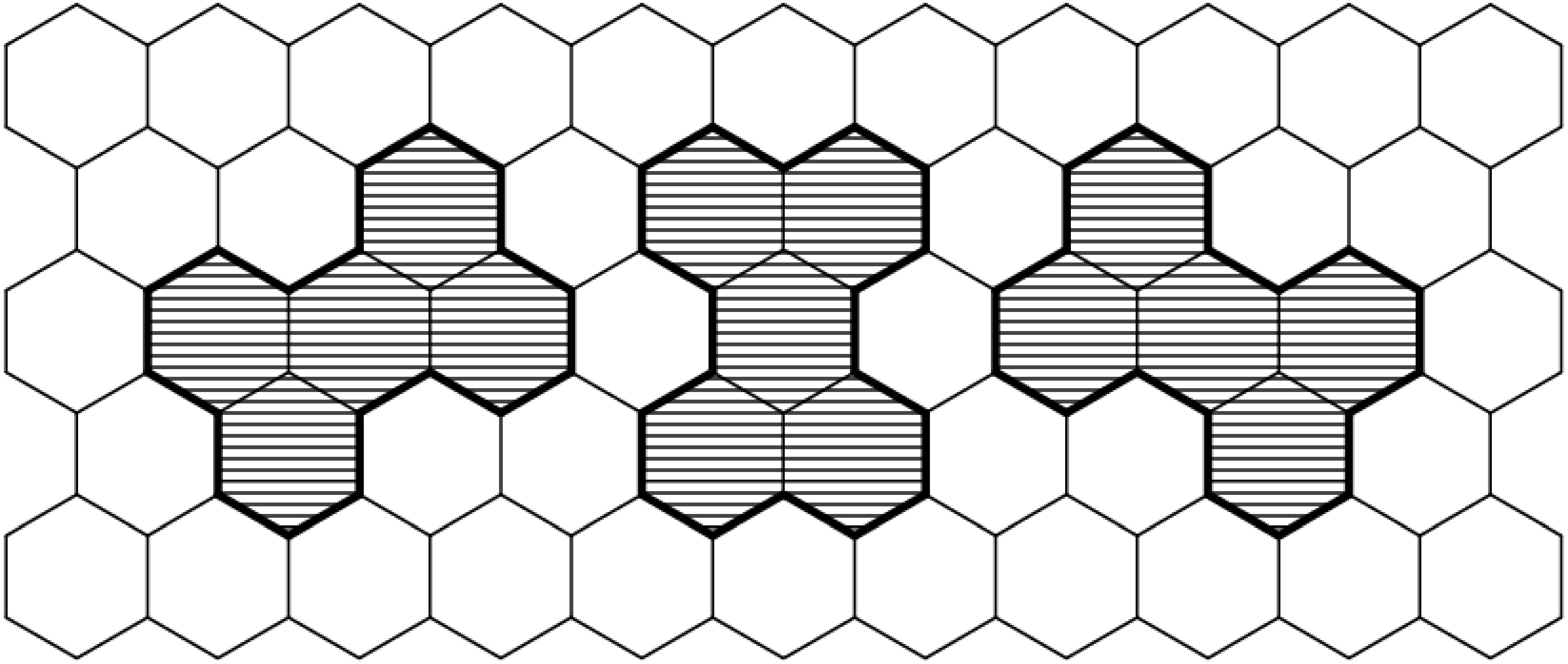
Advanced topic: Counting hexagonal systems

- Another point of view: a HS appers in three different orientations

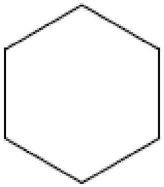


Advanced topic: Counting hexagonal systems

Example: |Aut(S)| = 4, so S appears in 3 = 12 / 4 different orientations

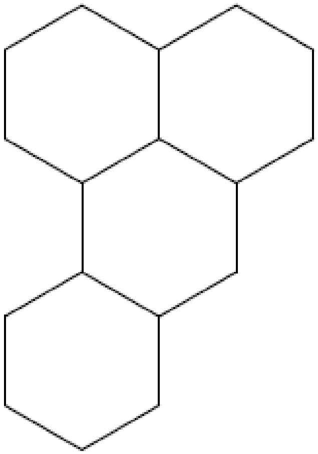


Advanced topic:
Counting hexagonal systems



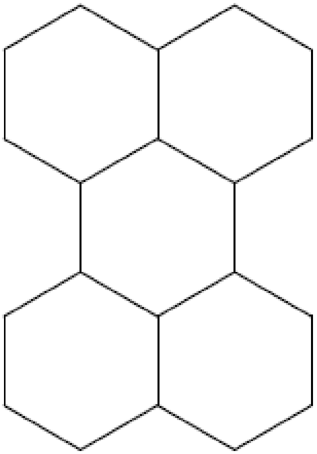
|Aut(S)| = 12

1 orientation



|Aut(S)| = 1

12 orientations



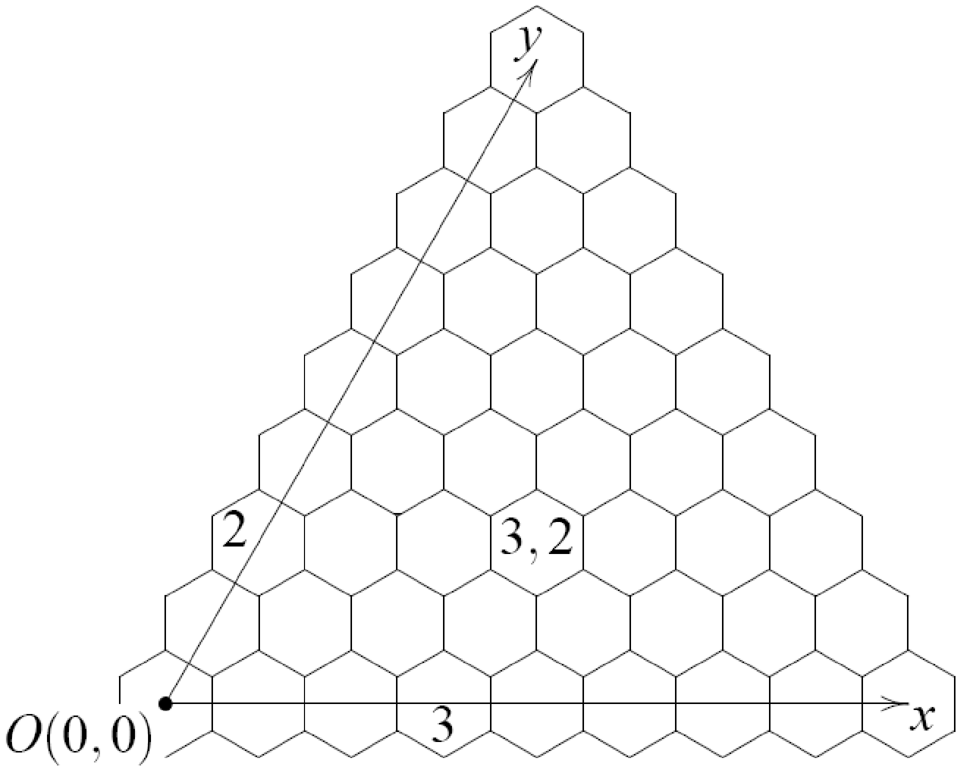
|Aut(S)| = 4

3 orientations

Advanced topic: Counting hexagonal systems

- The easiest way to handle a beast is to put it into a cage:

Cage(h)

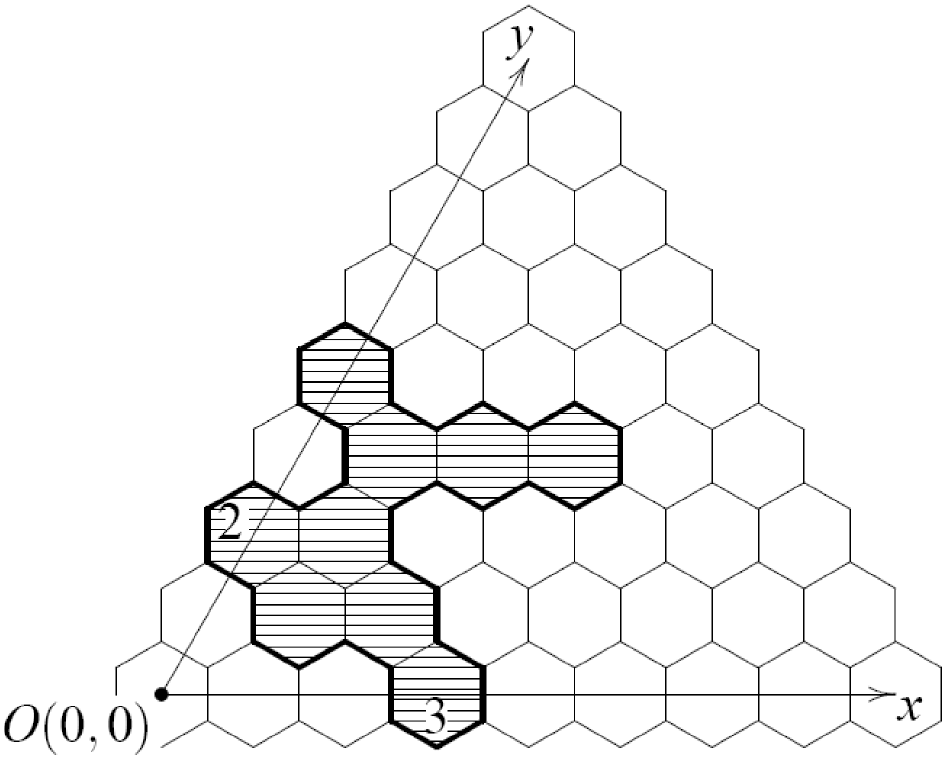


Advanced topic: Counting hexagonal systems

- A properly placed HS
- **Theorem.** Let *S* be a HS with *h* hex's. There are

  12 / |Aut(*S*)|

  different HSs which are isomorphic to *S* and properly placed in Cage(*h*).



Advanced topic: Counting hexagonal systems

Group	D_{6h}	C_{6h}	D_{3h}	C_{3h}	D_{2h}	C_{2h}	C_{2v}	C_s
Card.	12	6	6	3	4	2	2	1

Advanced topic: Counting hexagonal systems

Group	D_{6h}	C_{6h}	D_{3h}	C_{3h}	D_{2h}	C_{2h}	C_{2v}	C_s
Card.	12	6	6	3	4	2	2	1

- H(*h*) = #(**all** HS's with *h* hexagons)
- N(*h*) = #(**nonisomorphic** HS's with *h* hex's)
- N(*h*, *G*) = #(**nonisomorphic** HS's with *h* hex's whose Aut group is *G*)

Advanced topic: Counting hexagonal systems

Group	D_{6h}	C_{6h}	D_{3h}	C_{3h}	D_{2h}	C_{2h}	C_{2v}	C_s
Card.	12	6	6	3	4	2	2	1

- $N(h) = N(h, D_{6h}) + N(h, C_{6h}) + N(h, D_{3h}) + N(h, C_{3h}) + N(h, D_{2h}) + N(h, C_{2h}) + N(h, C_{2v}) + N(h, C_s)$
- $H(h) = N(h, D_{6h}) + 2N(h, C_{6h}) + 2N(h, D_{3h}) + 4N(h, C_{3h}) + 3N(h, D_{2h}) + 6N(h, C_{2h}) + 6N(h, C_{2v}) + 12N(h, C_s)$

Advanced topic: Counting hexagonal systems

Group	D_{6h}	C_{6h}	D_{3h}	C_{3h}	D_{2h}	C_{2h}	C_{2v}	C_s
Card.	12	6	6	3	4	2	2	1

- $N(h) = N(h, D_{6h}) + N(h, C_{6h}) + N(h, D_{3h}) + N(h, C_{3h}) + N(h, D_{2h}) + N(h, C_{2h}) + N(h, C_{2v}) + N(h, C_s)$
- $H(h) = N(h, D_{6h}) + 2N(h, C_{6h}) + 2N(h, D_{3h}) + 4N(h, C_{3h}) + 3N(h, D_{2h}) + 6N(h, C_{2h}) + 6N(h, C_{2v}) + 12N(h, C_s)$

Advanced topic: Counting hexagonal systems

Group	D_{6h}	C_{6h}	D_{3h}	C_{3h}	D_{2h}	C_{2h}	C_{2v}	C_s
Card.	12	6	6	3	4	2	2	1

- $N(h) = N(h, D_{6h}) + N(h, C_{6h}) + N(h, D_{3h})$
  $+ N(h, C_{3h}) + N(h, D_{2h}) + N(h, C_{2h})$
  $+ N(h, C_{2v}) + N(h, C_s)$
- $H(h) = N(h, D_{6h}) + 2N(h, C_{6h}) + 2N(h, D_{3h})$
  $+ 4N(h, C_{3h}) + 3N(h, D_{2h}) + 6N(h, C_{2h})$
  $+ 6N(h, C_{2v}) + 12N(h, C_s)$

Advanced topic: Counting hexagonal systems

Group	D_{6h}	C_{6h}	D_{3h}	C_{3h}	D_{2h}	C_{2h}	C_{2v}	C_s
Card.	12	6	6	3	4	2	2	1

- $N(h) = N(h, D_{6h}) + N(h, C_{6h}) + N(h, D_{3h}) + N(h, C_{3h}) + N(h, D_{2h}) + N(h, C_{2h}) + N(h, C_{2v}) + N(h, C_s)$
- $H(h) = N(h, D_{6h}) + 2N(h, C_{6h}) + 2N(h, D_{3h}) + 4N(h, C_{3h}) + 3N(h, D_{2h}) + 6N(h, C_{2h}) + 6N(h, C_{2v}) + 12N(h, C_s)$

Advanced topic: Counting hexagonal systems

- Implemented for IBM PC compatible computers in Modula-2
- Five modules and more than 1900 bruto program lines
- It has been used to determine the number of all properly placed hexagonal systems with at most 17 hexagons

Advanced topic: Counting hexagonal systems

- We had to divide the task into several smaller tasks (as the matter of fact, 197 smaller tasks)
- This made it possible to run the program on several sites: Novi Sad, Ottawa and Trondheim.
- The parallelization was performed by hand