

A company cannot spend anymore than 120 hours per week making toys and 160 hours per week finishing toys.

|            | <b>Sell</b> | <b>Materials</b> | <b>Make (hours)</b> | <b>Finish (hours)</b> | <b>Max sold</b> |
|------------|-------------|------------------|---------------------|-----------------------|-----------------|
| Plane (X1) | \$12        | \$4              | 3                   | 1                     | 30              |
| Boat (X2)  | \$10        | \$3              | 1                   | 2                     | --              |

Maximize  $8 X1 + 7 X2$

subject to

$$3 X1 + 1 X2 \leq 120$$

$$1 X1 + 2 X2 \leq 160$$

$$1 X1 + 0 X2 \leq 30$$

$$X1, X2 \geq 0$$

Solution: (16, 72)

Solve for  $y$  using complementary slackness then give an economic interpretation of the dual variables.

After 3 pivots:

$$X2 = 72 + 0.20 X3 - 0.60 X4$$

$$X5 = 14 + 0.40 X3 - 0.20 X4$$

$$X1 = 16 - 0.40 X3 + 0.20 X4$$

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$$z = 632 - 1.80 X3 - 2.60 X4$$

One more making hour: \$1.80.

One more finishing hour: \$2.60

It would not help to be able to sell more planes.

What are B and  $B^{-1}$ ?

Maximize  $8 X_1 + 7 X_2$

subject to

$$3 X_1 + 1 X_2 \leq 120$$

$$1 X_1 + 2 X_2 \leq 160$$

$$1 X_1 + 0 X_2 \leq 30$$

$$X_1, X_2 \geq 0$$

Use last dictionary to get  $B^{-1}$ :

$$X_2 = 72 + 0.2 X_3 - 0.6 X_4$$

$$X_5 = 14 + 0.4 X_3 - 0.2 X_4$$

$$X_1 = 16 - 0.4 X_3 + 0.2 X_4$$

$$B = \begin{array}{c} X_2 \quad X_5 \quad X_1 \\ \begin{bmatrix} 1 & 0 & 3 \\ 2 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix} \end{array}$$

$$B^{-1} = \begin{array}{c} X_3 \quad X_4 \quad X_5 \\ \begin{bmatrix} -0.2 & 0.6 & 0 \\ -0.4 & 0.2 & 1 \\ 0.4 & -0.2 & 0 \end{bmatrix} \end{array}$$

Maximize  $8 X1 + 7 X2$

subject to

$$\begin{aligned} 3 X1 + 1 X2 &\leq 120 + t1 && // \text{making} \\ 1 X1 + 2 X2 &\leq 160 + t2 && // \text{finishing} \\ 1 X1 + 0 X2 &\leq 30 + t3 && // \text{max planes} \\ X1, X2 &\geq 0 \end{aligned}$$

$$\begin{bmatrix} X2 \\ X5 \\ X1 \end{bmatrix} = B^{-1} b = \begin{bmatrix} -0.2 & 0.6 & 0 \\ -0.4 & 0.2 & 1 \\ 0.4 & -0.2 & 0 \end{bmatrix} \begin{bmatrix} 120 + t1 \\ 160 + t2 \\ 30 + t3 \end{bmatrix}$$

$$X2 = 72 - 0.2 t1 + 0.6 t2 // \text{boats}$$

$$X5 = 14 - 0.4 t1 + 0.2 t2 + t3$$

$$X1 = 16 + 0.4 t1 - 0.2 t2 // \text{planes}$$

## Announcements:

CSC 545 only:

Survey Paper- due on Fri. Oct. 17 at 11:55pm.

Accepted until Tues. Oct. 21 at 11:55pm with a 10% late penalty.

Make sure you use 12 point font, at least 1.5 spacing and your .pdf file is uploaded.

## Both classes:

Programming project 2:

Due at 11:55pm on Fri. Oct. 24.

Accepted with 10% penalty until Tues. Oct. 28 at 11:55pm.

Two applications of linear programming to chemistry:

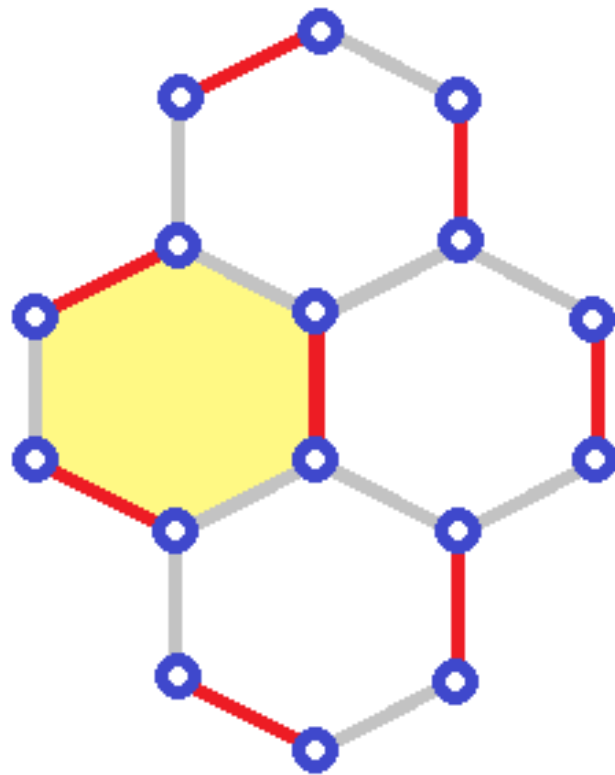
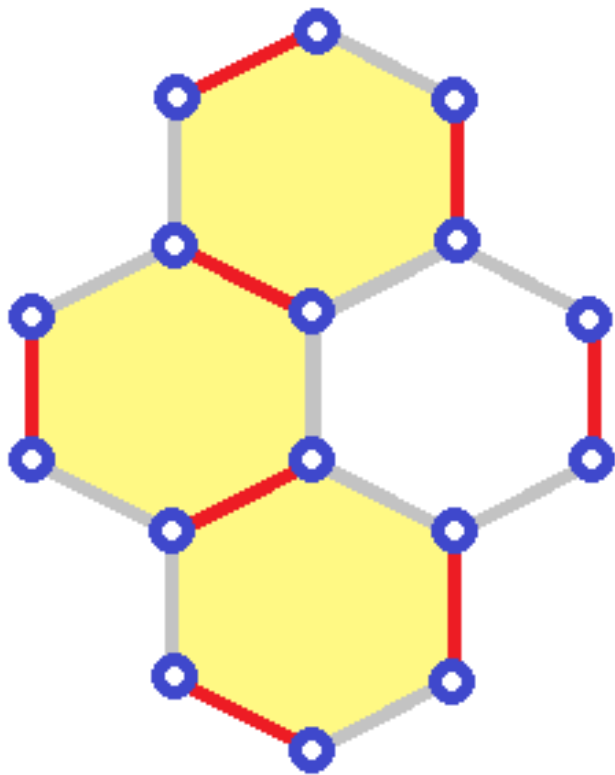
Finding the Clar number and the Fries number of a benzenoid in polynomial time using a LP.

The desired solutions are integer but it has been proven that the basic feasible solutions are all integral so integer programming tactics are not required.

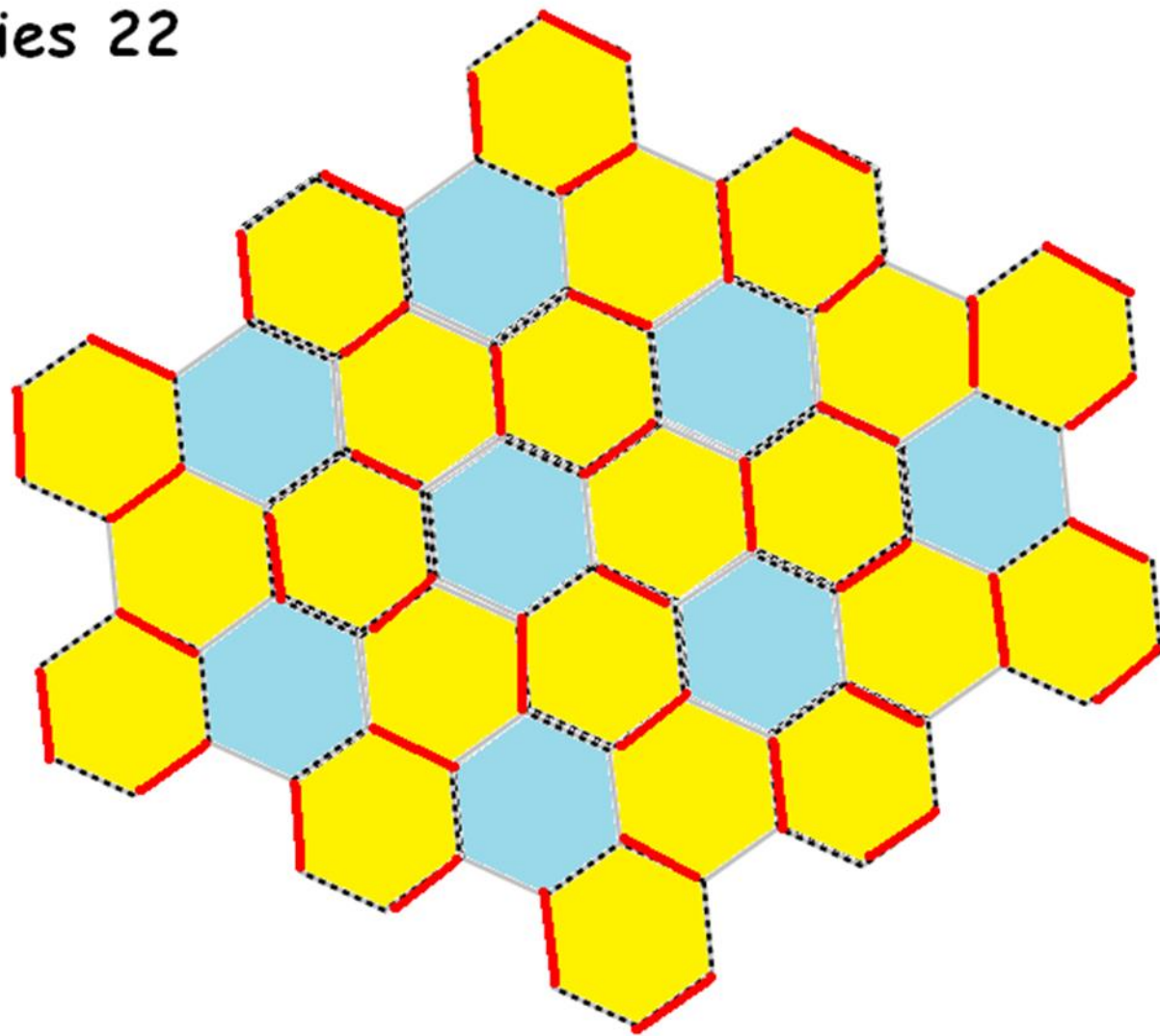
**Matching:** collection of disjoint edges.

**Benzenoid hexagon:** hexagon with 3 matching edges.

**Fries number:** maximum over all perfect matchings of the number of benzenoid hexagons.



Fries 22

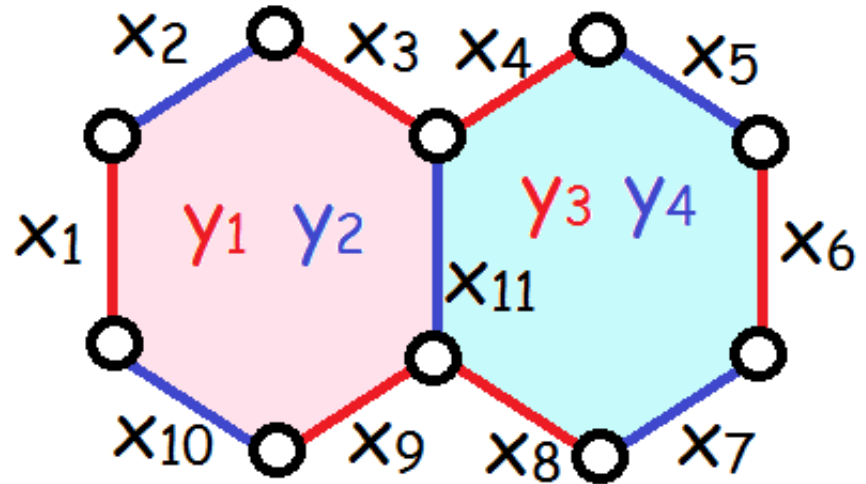




Proof that the solutions to the LP are integral:

```
@ARTICLE{LP_Fries,  
author = {Hernan G. Abeledo and Gary  
W. Atkinson},  
title = {Polyhedral Combinatorics of  
Benzenoid Problems},  
journal = {Lect. Notes Comput. Sci},  
year = {1998},  
volume = {1412},  
pages = {202--212}  
}
```

One variable  $x_e$   
 for each edge  $e$ .  
 Two variables per  
 hexagon.  
 All variables are  
 constrained to be  
 between 0 and 1.



- $y_1 = 1$  pink hex. is benzenoid because of red edges.
- $y_2 = 1$  pink hex. is benzenoid because of blue edges.
- $y_3 = 1$  aqua hex. is benzenoid because of red edges.
- $y_4 = 1$  aqua hex. is benzenoid because of blue edges.

Maximize  $y_1 + y_2 + y_3 + y_4$

Maximize  $y_1 + y_2 + y_3 + y_4$

To get a perfect matching:

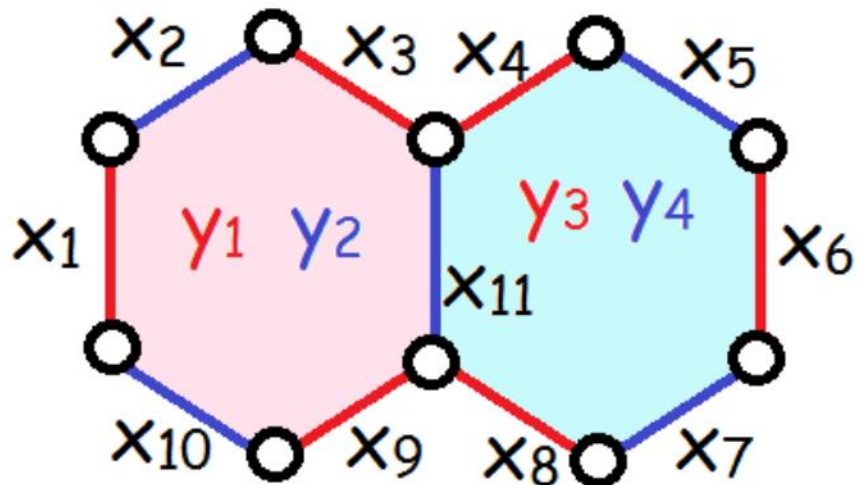
For each vertex, the number of edges incident sums to 1:

$$x_1 + x_2 = 1$$

$$x_2 + x_3 = 1$$

$$x_3 + x_4 + x_{11} = 1$$

...



## To ensure benzenoid hexagons:

Red edges of pink:

$$x_1 - \gamma_1 \geq 0$$

$$x_3 - \gamma_1 \geq 0$$

$$x_9 - \gamma_1 \geq 0$$

Blue edges of pink:

$$x_2 - \gamma_2 \geq 0$$

$$x_{10} - \gamma_2 \geq 0$$

$$x_{11} - \gamma_2 \geq 0$$

Red edges of aqua:

$$x_4 - \gamma_3 \geq 0$$

$$x_6 - \gamma_3 \geq 0$$

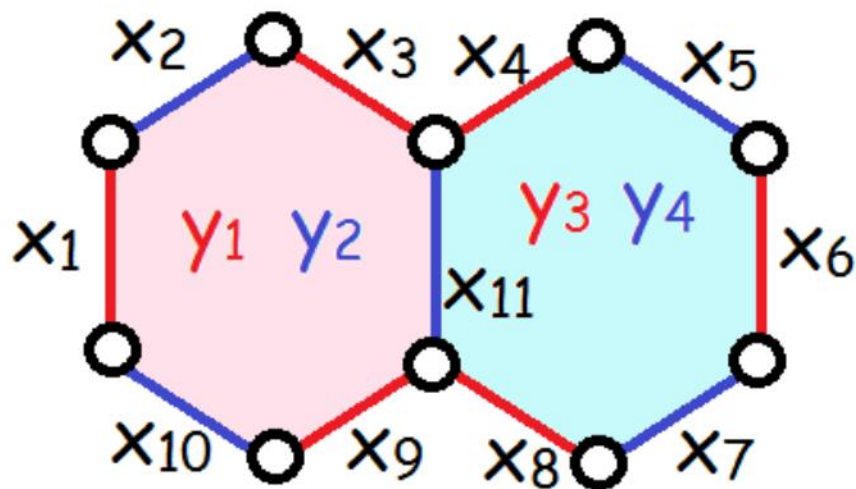
$$x_8 - \gamma_3 \geq 0$$

Blue edges of aqua:

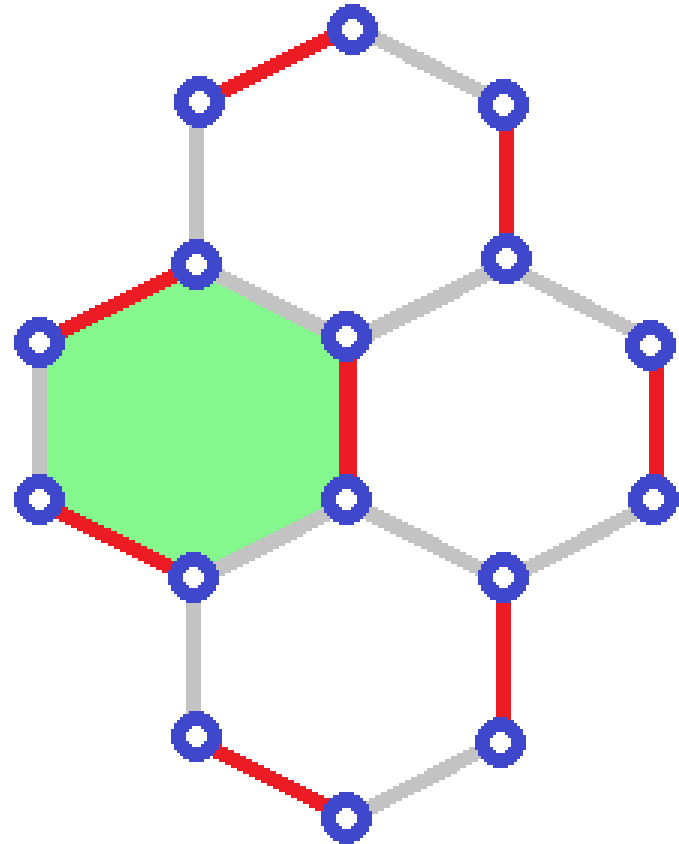
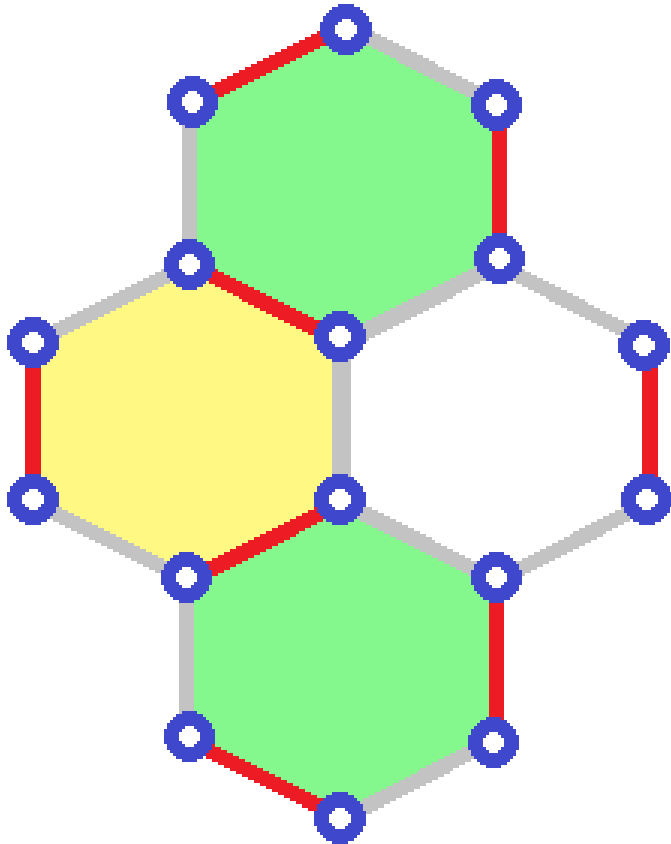
$$x_5 - \gamma_4 \geq 0$$

$$x_7 - \gamma_4 \geq 0$$

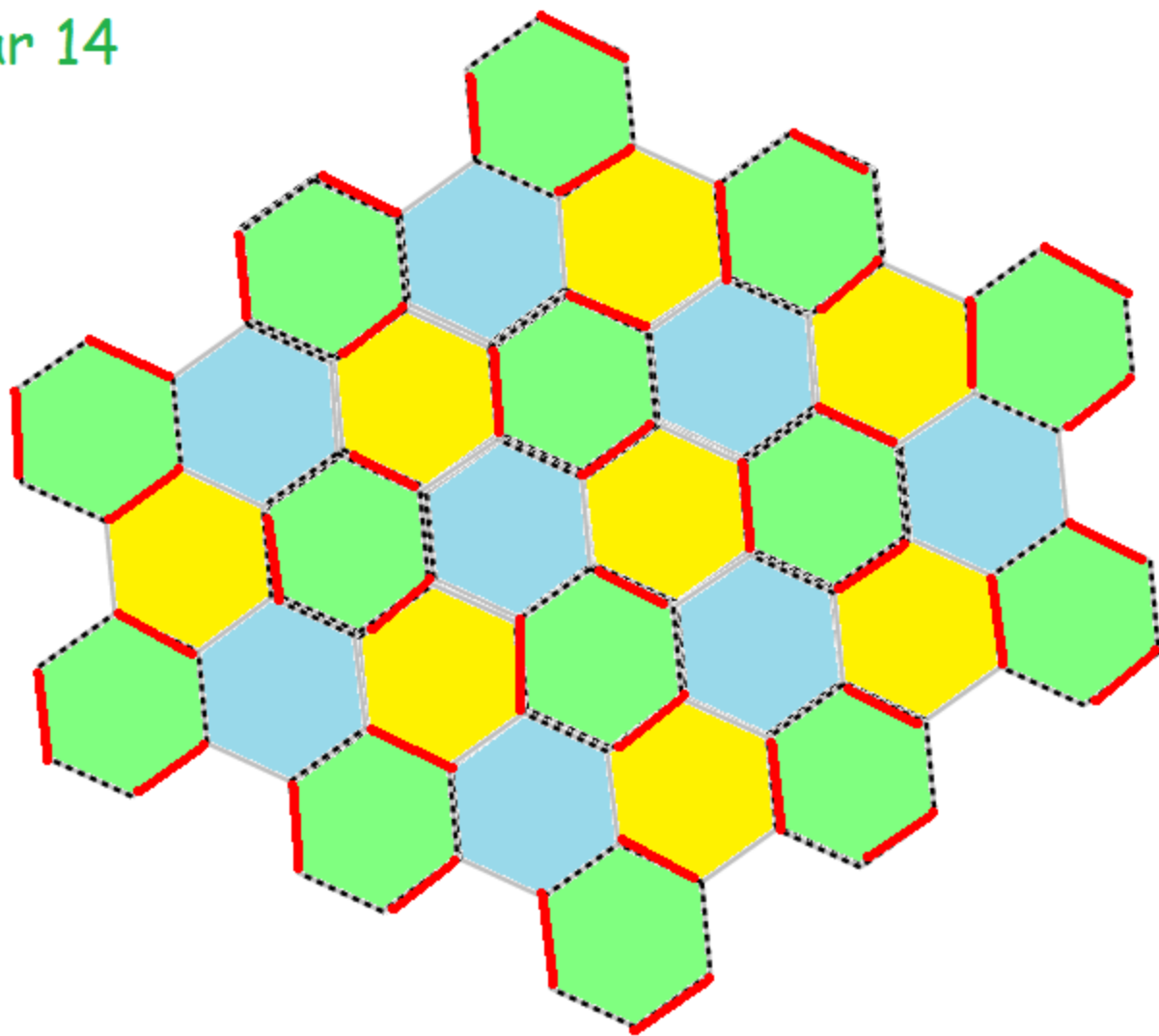
$$x_{11} - \gamma_4 \geq 0$$

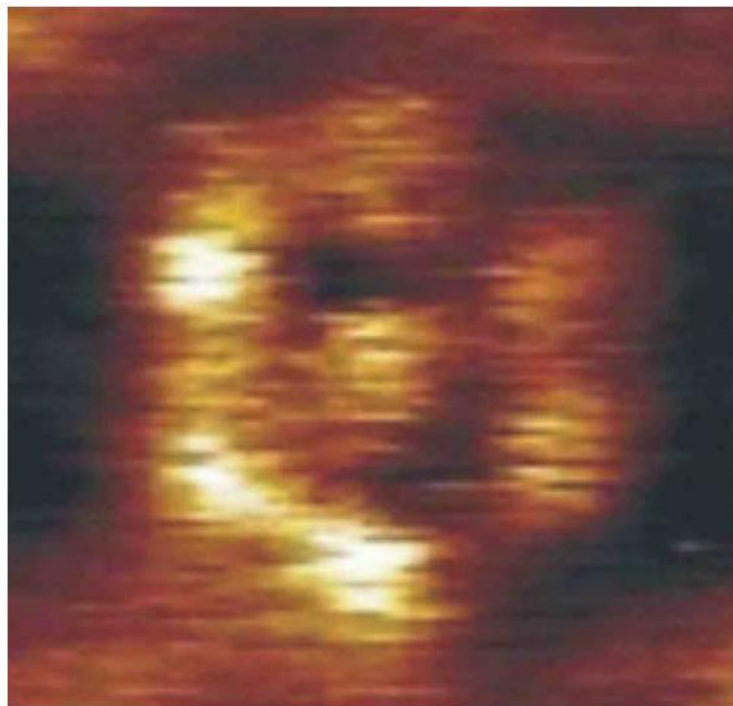


**Clar number:** maximum over all perfect matchings of the number of independent benzenoid hexagons.

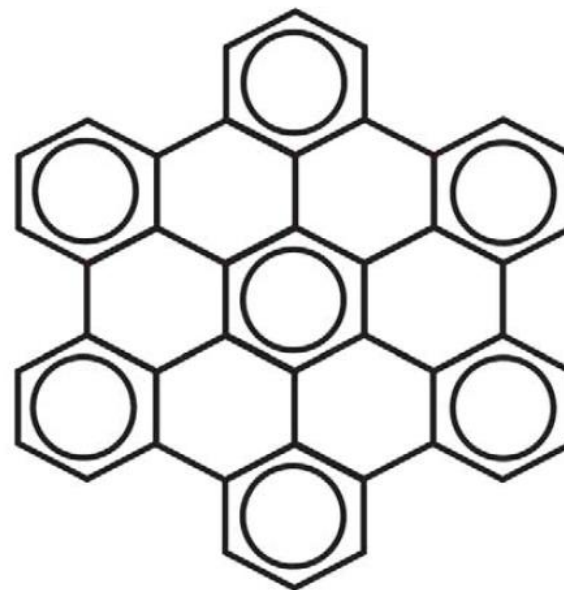


Clar 14





1 nm

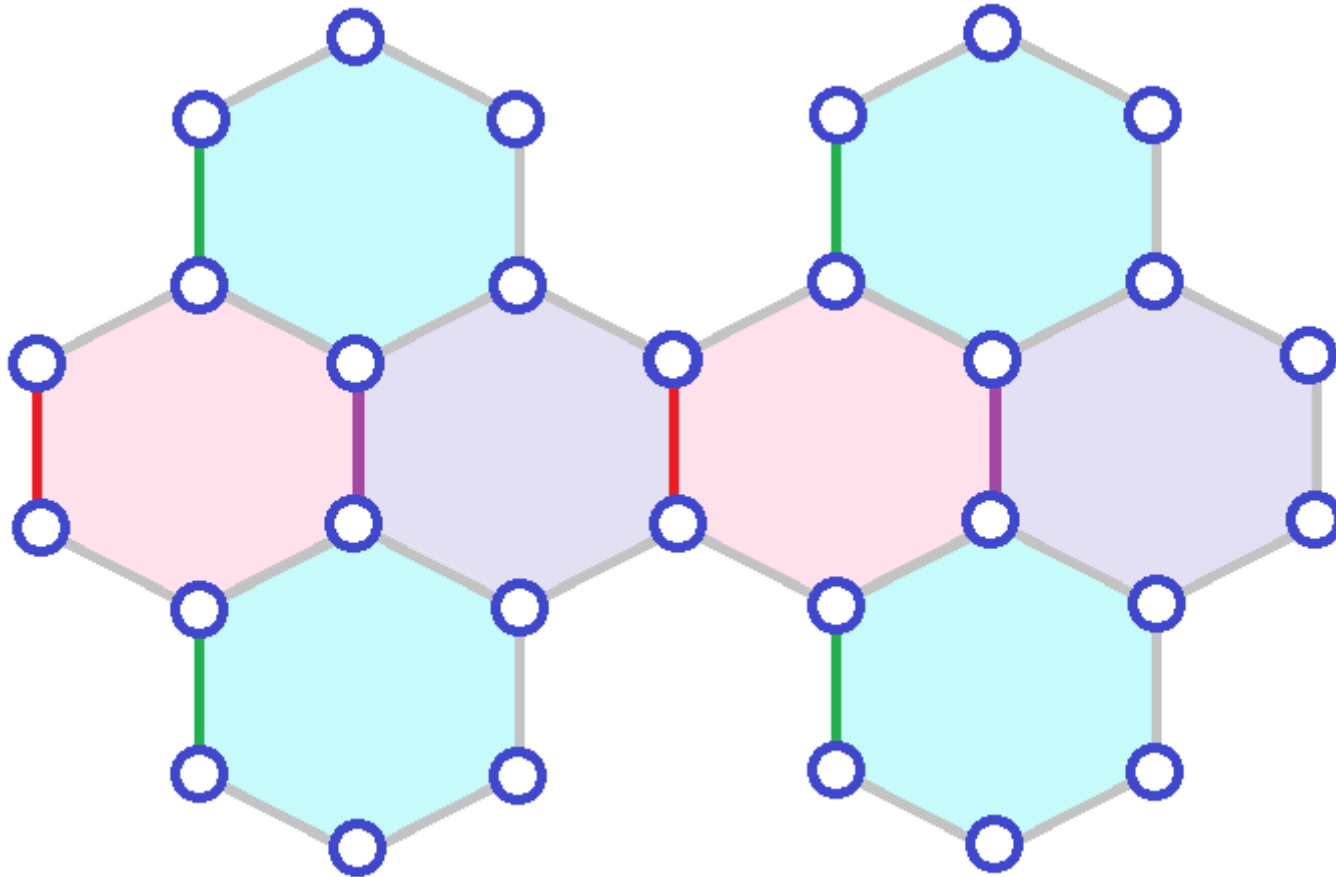


## Scanning Tunnelling Microscopy image of hexabenzocoronene

*from*

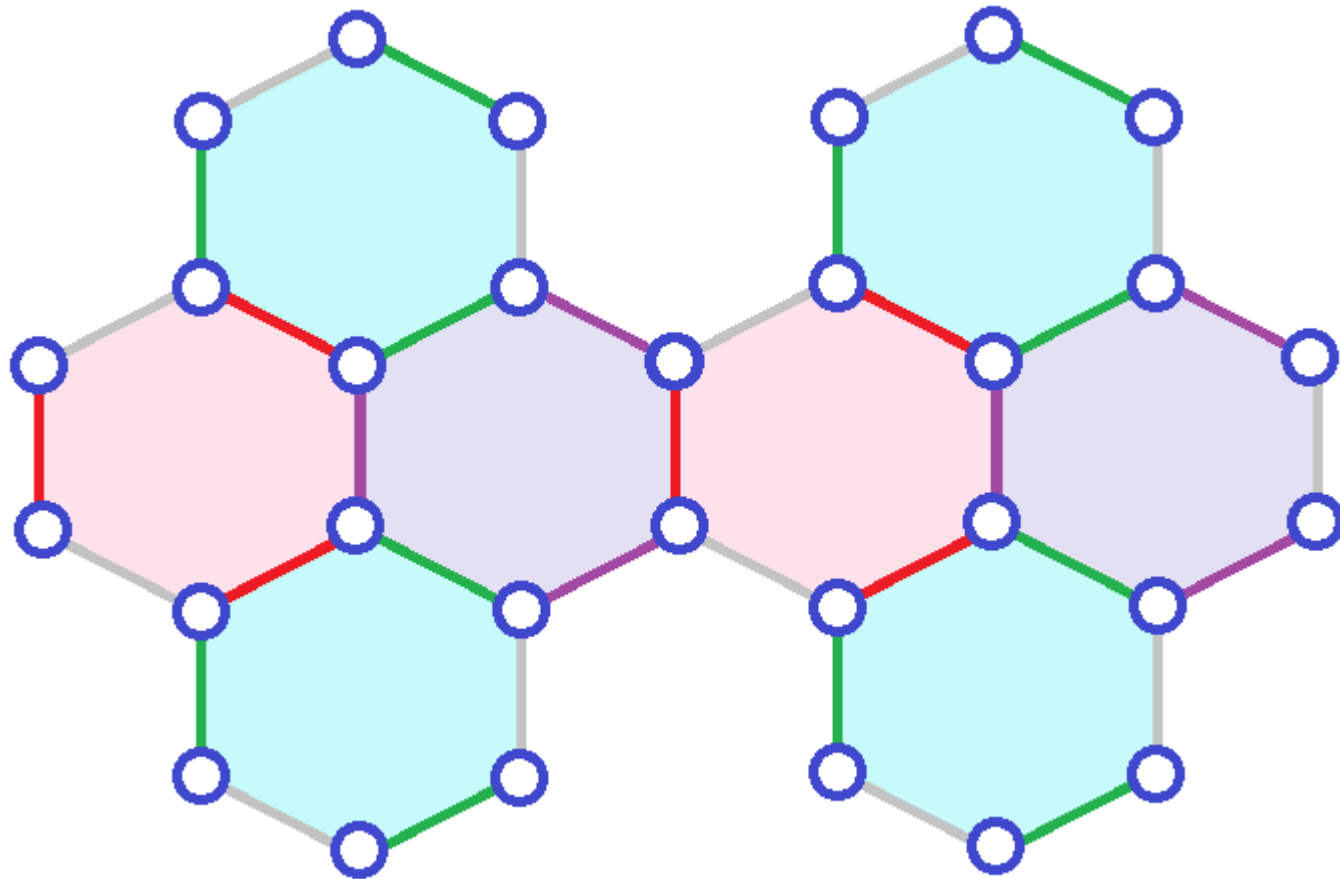
I Gutman, Ž Tomović, K Müllen, J P Rabe,  
Chemical Physics Letters 397 (2004) 412–416

LP for the Clar number: The LH edge of each hexagon is its **canonical edge**.

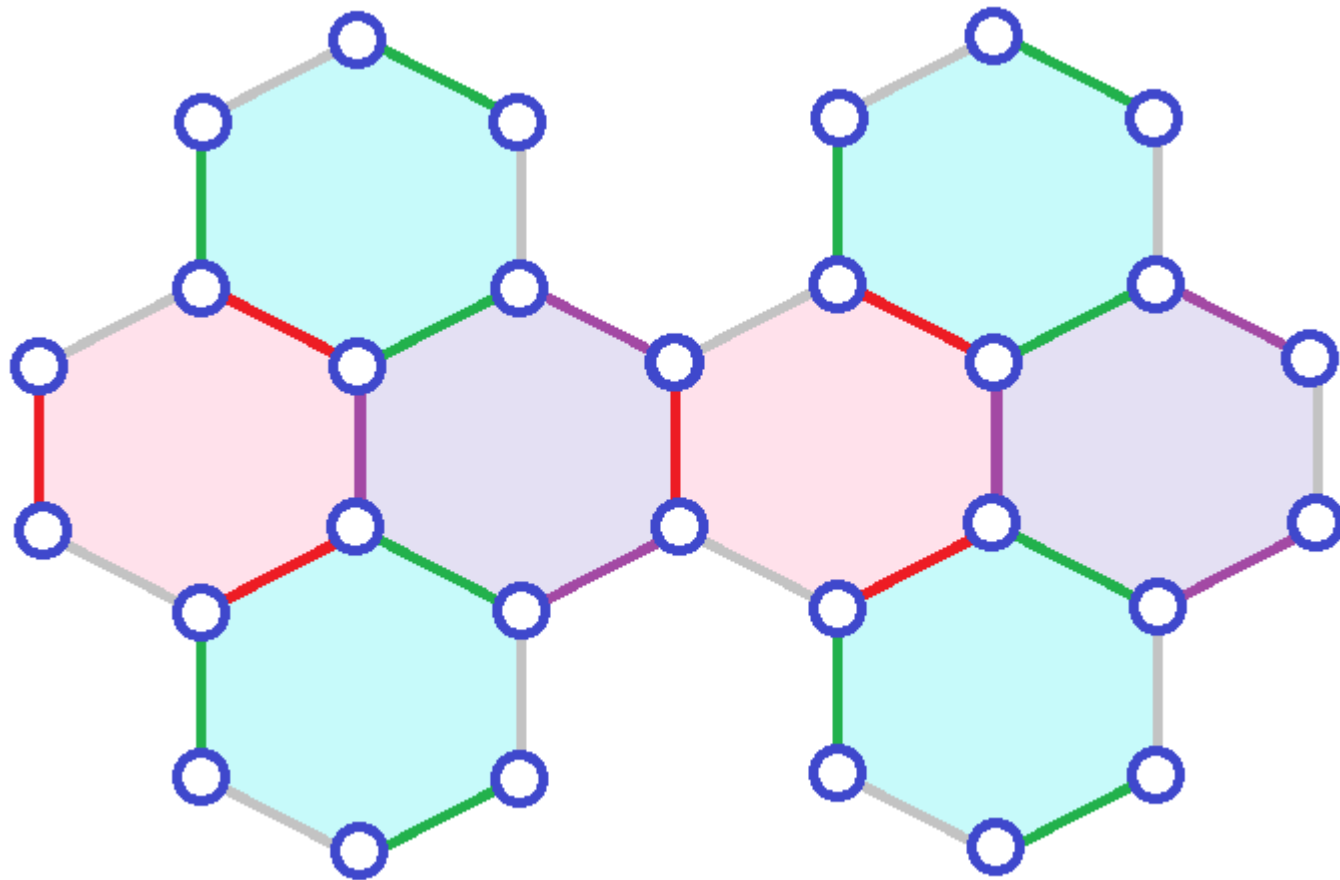




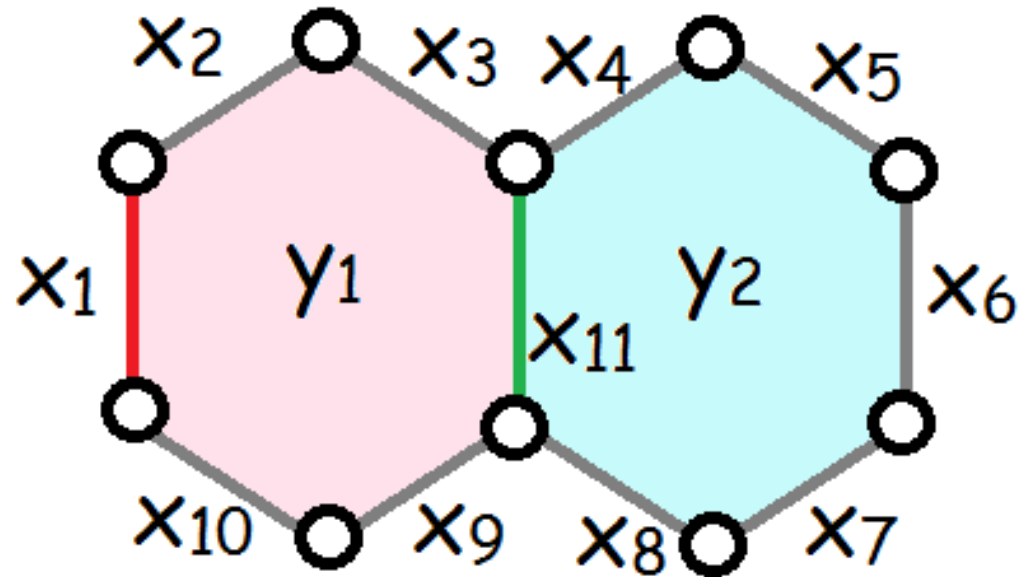
The corresponding matching is the **canonical matching** for the hexagon.



If a hexagon is *Clar*, assume it realizes its canonical matching.



Two variables  $x_e$ ,  $z_e$  for each edge  $e$ .  
 One variable  $y_h$  for each hexagon  $h$ .  
 All variables are constrained to be between 0 and 1.



$z_e = 1$  if  $e$  is a perfect matching edge.

$x_e = 1$  if  $e$  is a matching edge not in a benzenoid hexagon.

$y_h = 1$  if  $h$  is an independent benzenoid hexagon and 0 otherwise.

Maximize  $y_1 + y_2$

To get a perfect matching:

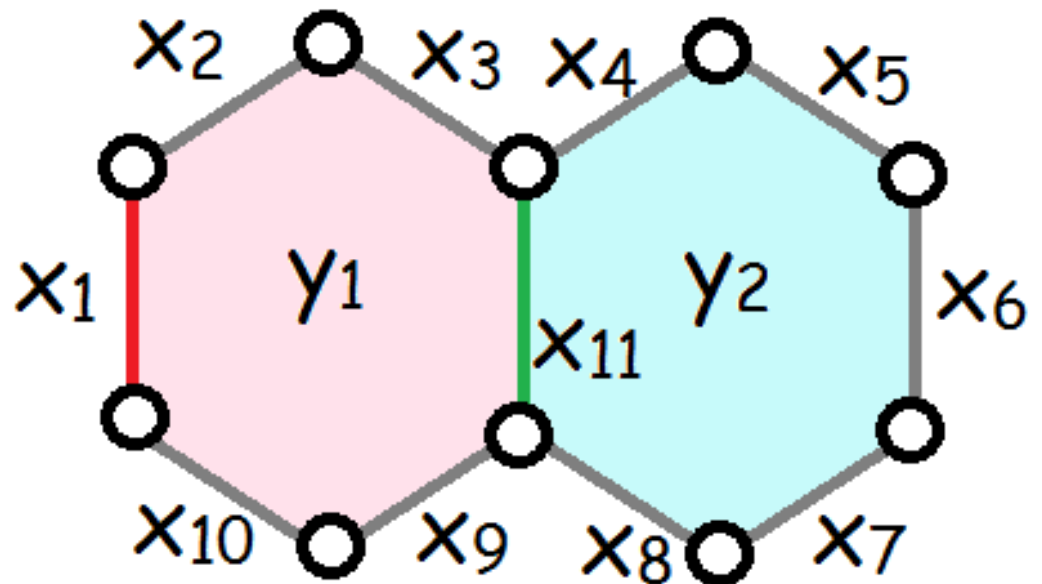
For each vertex, the number of edges incident sums to 1:

$$z_1 + z_2 = 1$$

$$z_2 + z_3 = 1$$

$$z_3 + z_4 + z_{11} = 1$$

...



To get the independent benzenoid hexagons:

For the pink hexagon:

$$x_1 + y_1 - z_1 = 0$$

$$x_3 + y_1 - z_3 = 0$$

$$x_9 + y_1 - z_9 = 0$$

If  $y_1 = 1$  then

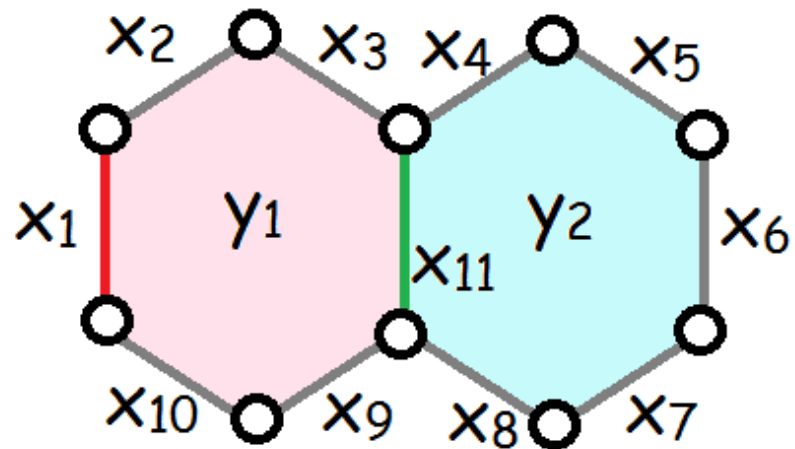
$$z_1 = z_3 = z_9 = 1 \Rightarrow$$

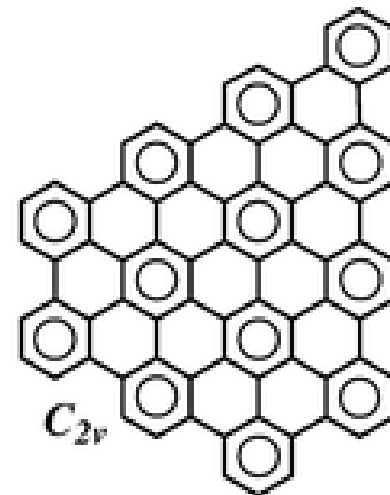
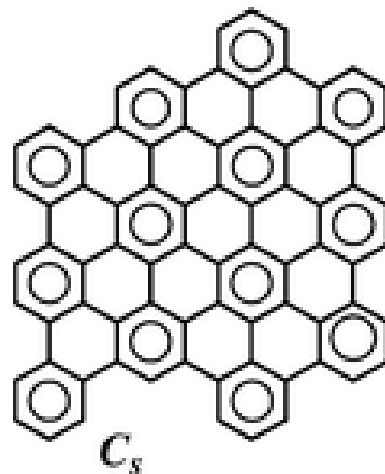
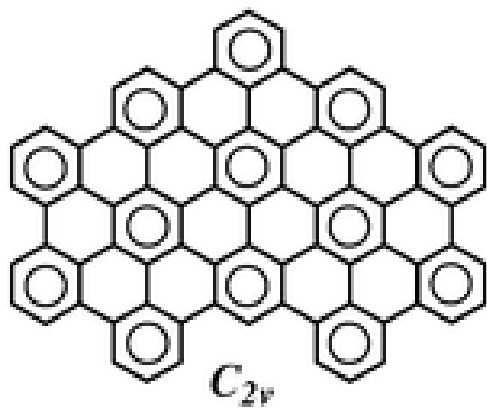
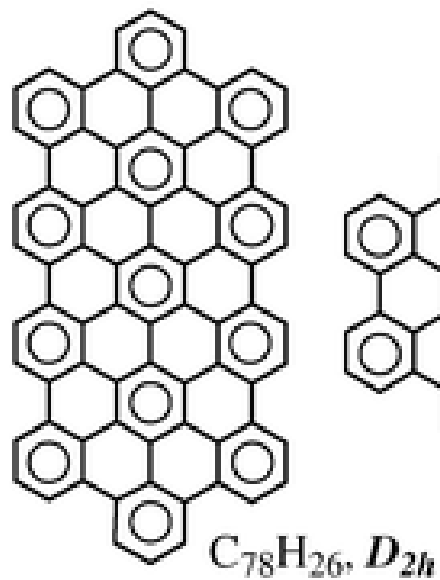
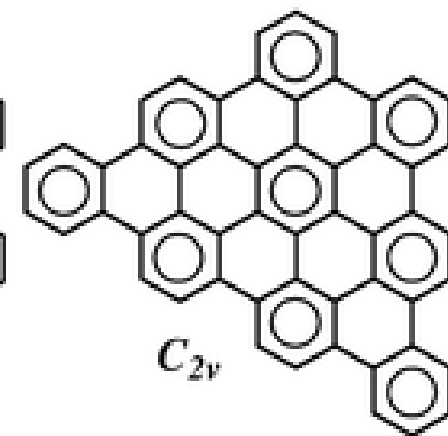
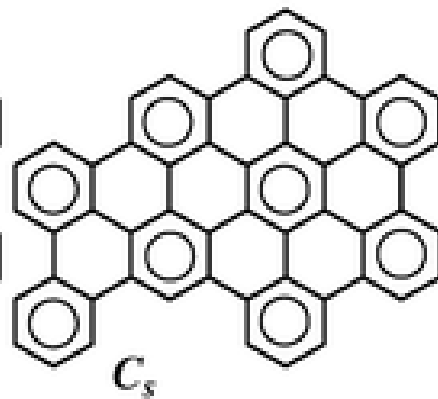
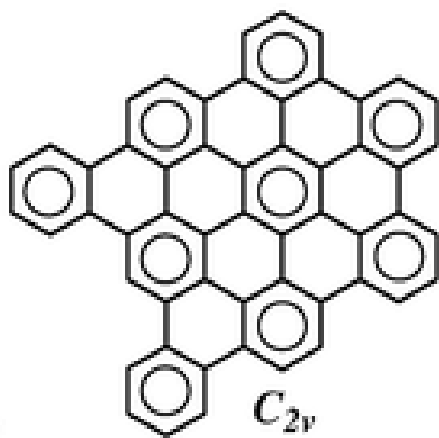
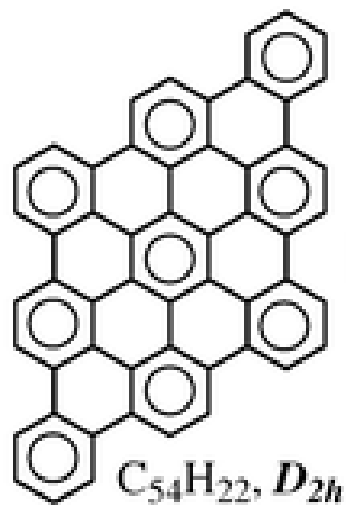
$$z_2 = z_{11} = z_{10} = 0$$

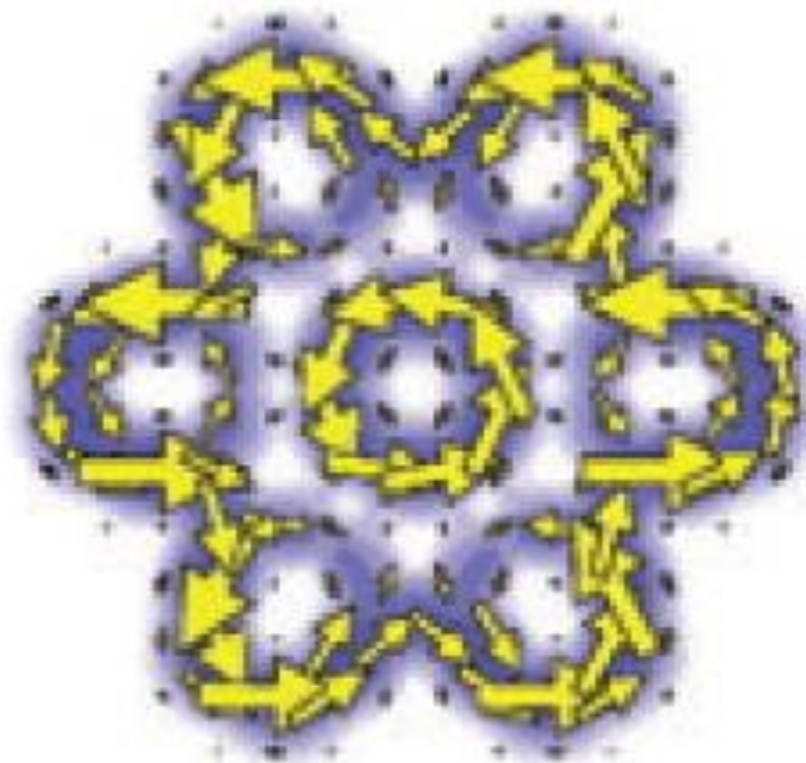
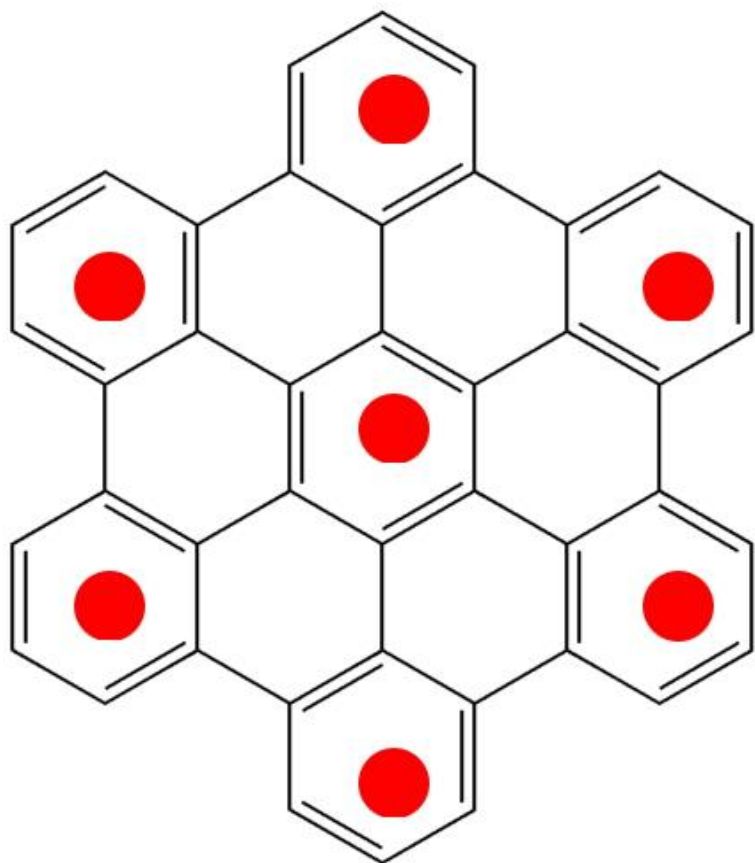
If  $y_1 = 1, y_2 = 0$

since

$$x_{11} + y_2 - z_{11} = 0$$







It's possible to find the Fries number and the Clar number using linear programming.



This is an example of a problem that is an integer programming problem where the integer solution magically appears when solving the linear programming problem.