Efficient Counting of the Number of Independent Sets on Polygonal Trees

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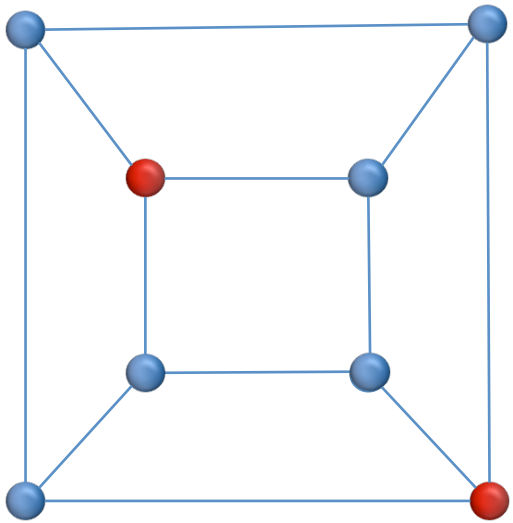
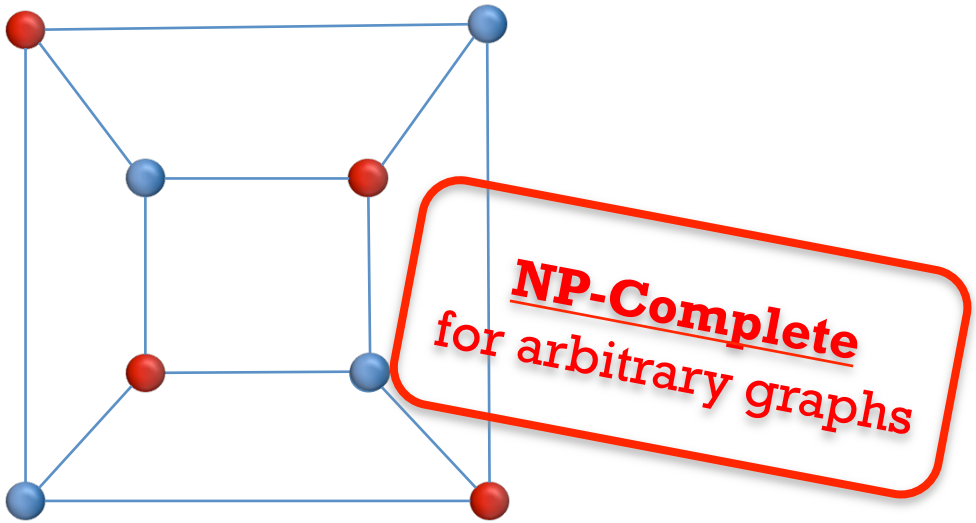
What is an independent set?

- In graph theory, an ***independet set*** is a set of vertices of a graph *G*, where any pair of them are adjacents in *G*.



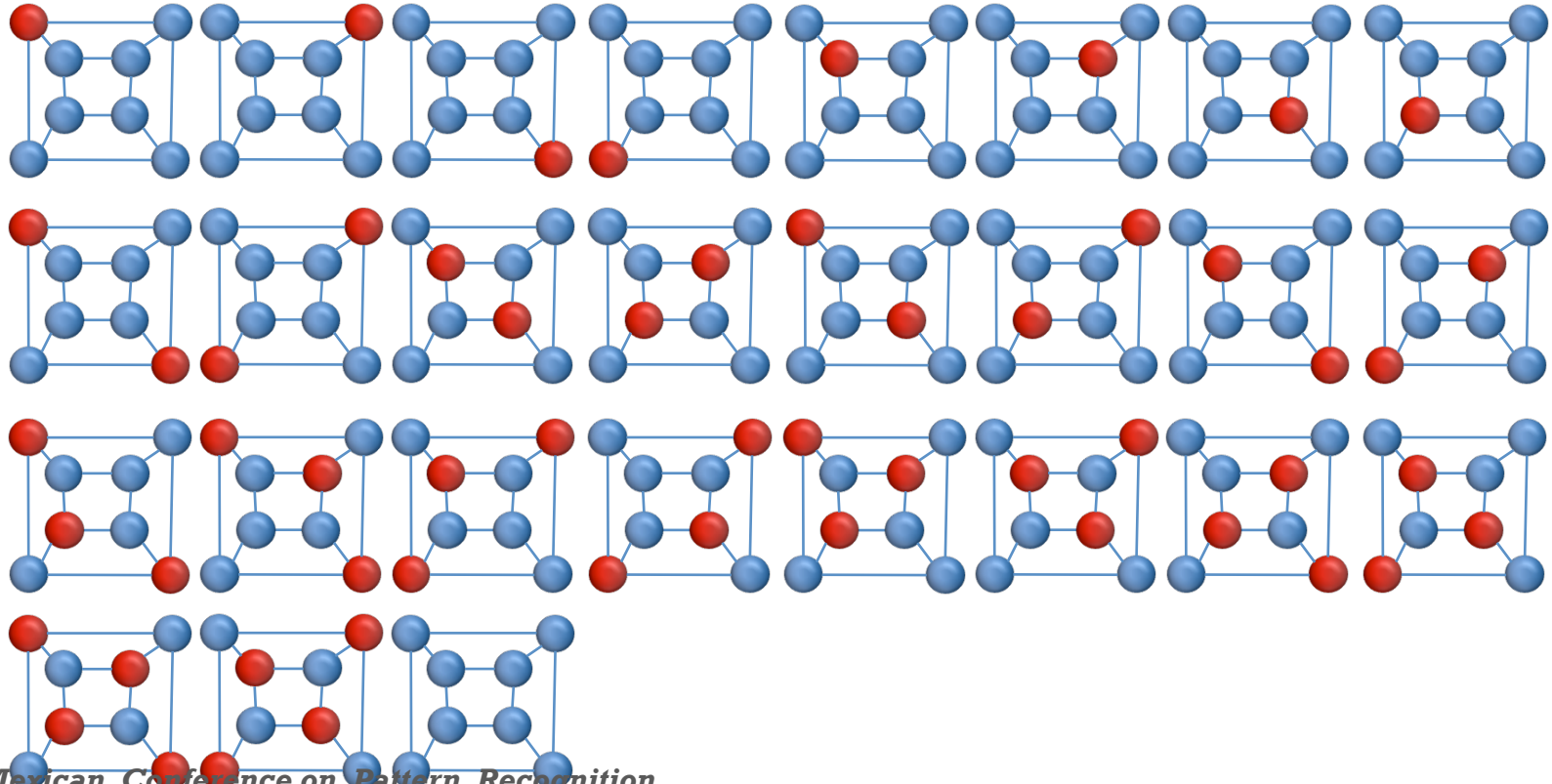
What is an independent set?

- The ***maximum independent set*** is the independent set of maximum cardinality.



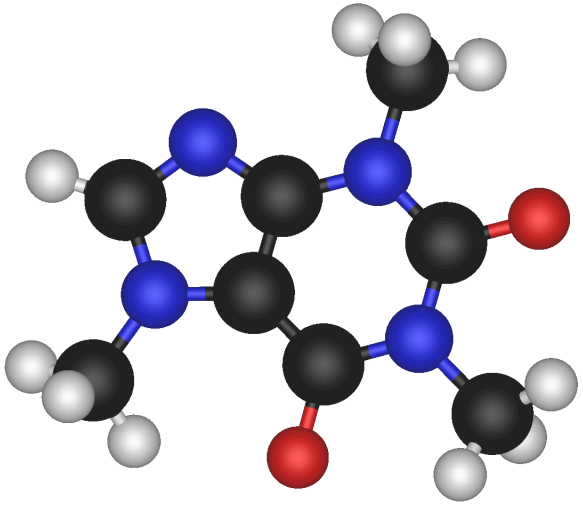
What is an independent set?

- The ***number of independent sets*** refers to, how many differents idependent set does *G* has?



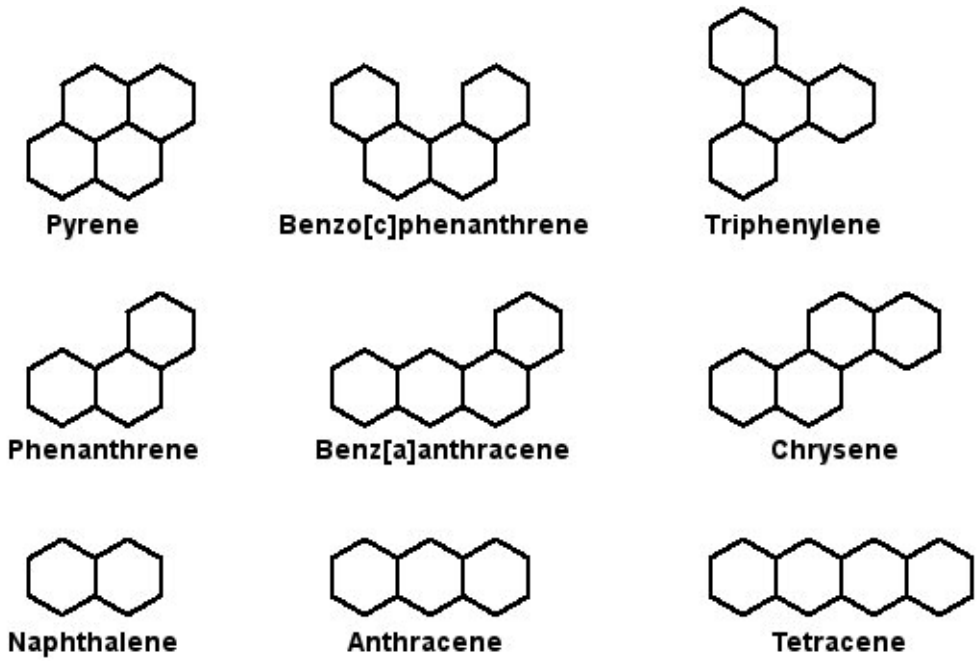
Motivation

- In mathematical chemistry, a ***molecular graph*** is a representation of the structural formula of a chemical compound in terms of graph theory.



Motivation

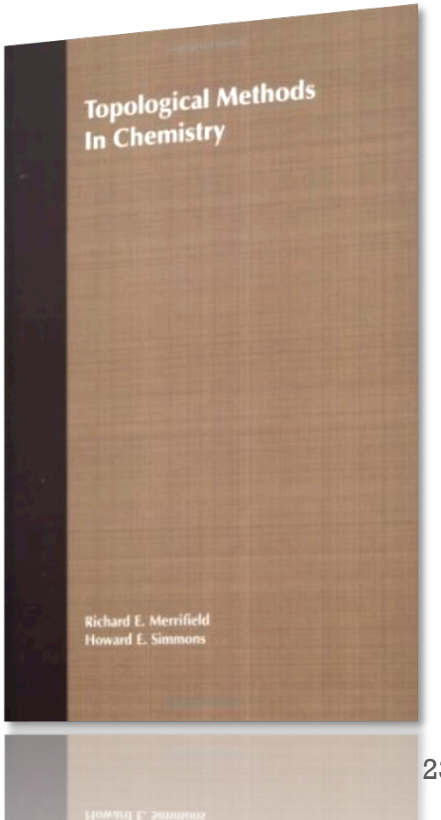
- For instance phenylene, poly-phenylyne and berzenoids has a particular structural patterns (polygonal graphs).



Motivation

- This molecular graphs presents a few intereting invariants like:
  - Hosoya index
  - Merrifield-Simmons index

The Merrifield-Simmons index was introduced by Merrifield and Simmons in 1989, they are one of the topological indices whose mathematical properties turned out to be applicable to several questions of molecular chemistry.



Motivation

- The definition of the Merrifiel-Simmons index:

$$\sum_{k\geq 0}^{n} ms(G,k)$$

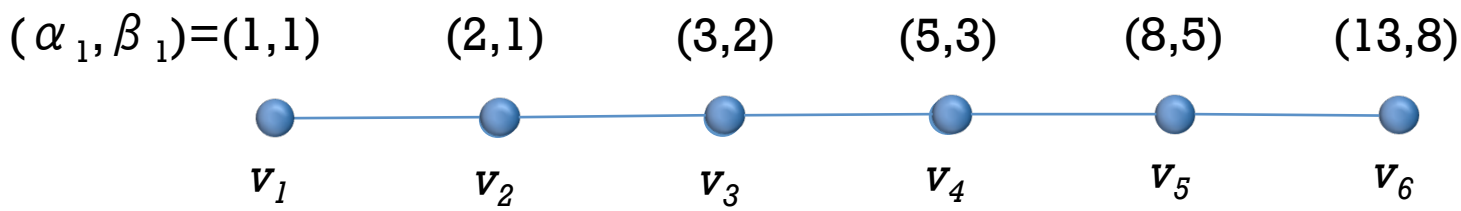
- Where ***ms(G,k)***, is the number of ways in which k mutually independent vertices can be chosen in G.

What do we know about *NI(G)*?

- The bad news ☹
  - Countig the number of independet sets is NP-Complete, even on 3-regular graphs.
- The good news!, there are polynomial algoritthms for:
  - Chordal graphs.
  - Grid graphs.
  - There is known extremal values for a few more families.
  - **And ☺ we present (now) a new way to compute *NI(G)* over polygonal trees.**

Counting the $NI(P_6)$

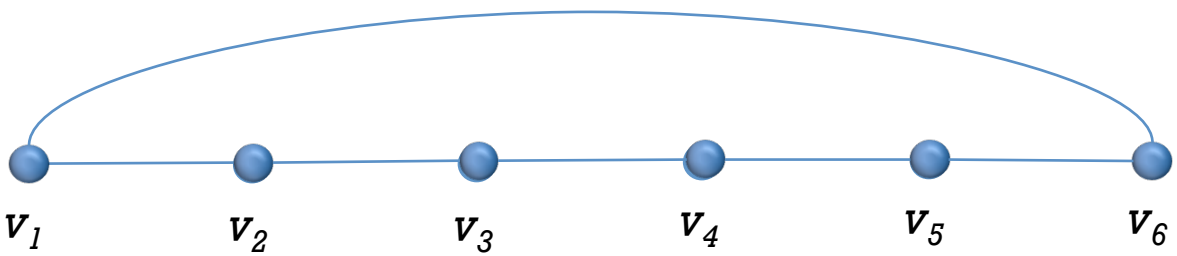
- Counting the $NI(P_6)$ with the Fibonacci recurrence.
  - We initialize $(\alpha_1, \beta_1)=(1,1)$
  - α_i denotes the $NI(P_i)$ where v_i does not participates.
  - β_i denotes the $NI(P_i)$ where v_i participates.
  - $(\alpha_i, \beta_i) = (\alpha_{i-1} + \beta_{i-1}, \alpha_{i-1})$



$$NI(P_6) = \alpha_6 + \beta_6 = 21$$

Counting the $NI(C_6)$

- Counting the $NI(C_6)$ with the Fibonacci recurrence.

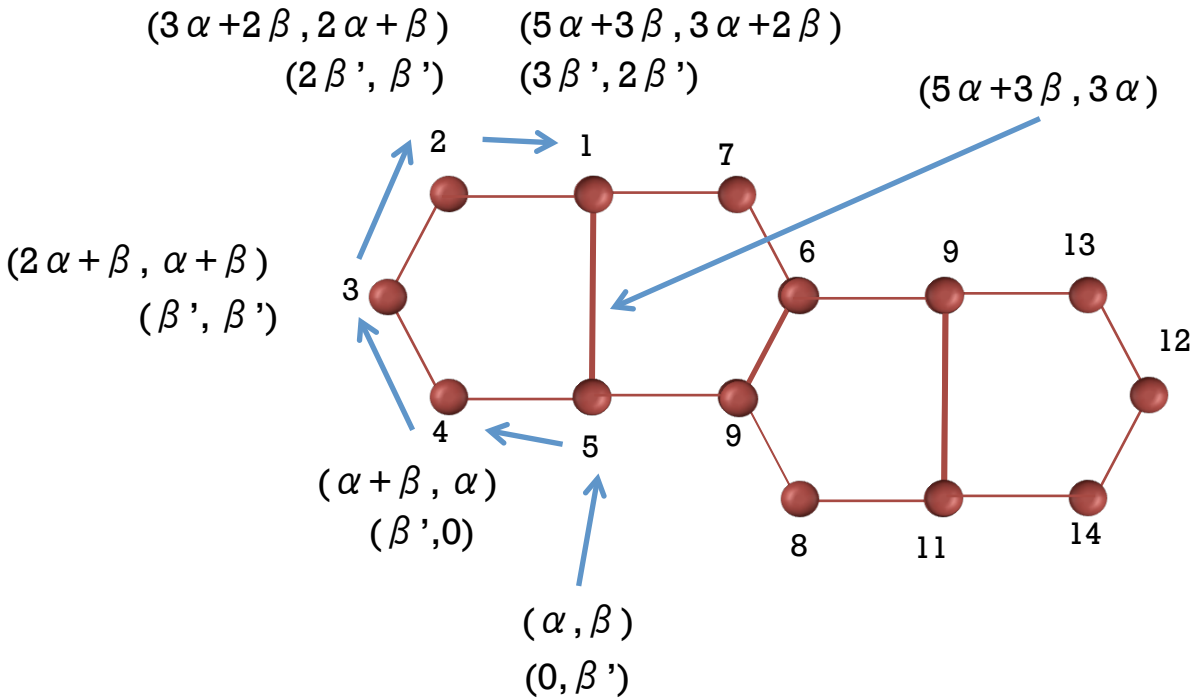


$(\alpha_1, \beta_1)=(1,1)$	(2,1)	(3,2)	(5,3)	(8,5)	(13,8)	(13,8)
$(\alpha'_1, \beta'_1)=(0,1)$	(1,0)	(1,1)	(2,1)	(3,2)	(5,3)	(X,3)
						(13,5)

$NI(P_6) = 18$

The Merrifield-Simmons index of *Pentalene*

- Pentalene (Pl) is a polycyclic hydrocarbon composed of two fused cyclopentadiene rings.



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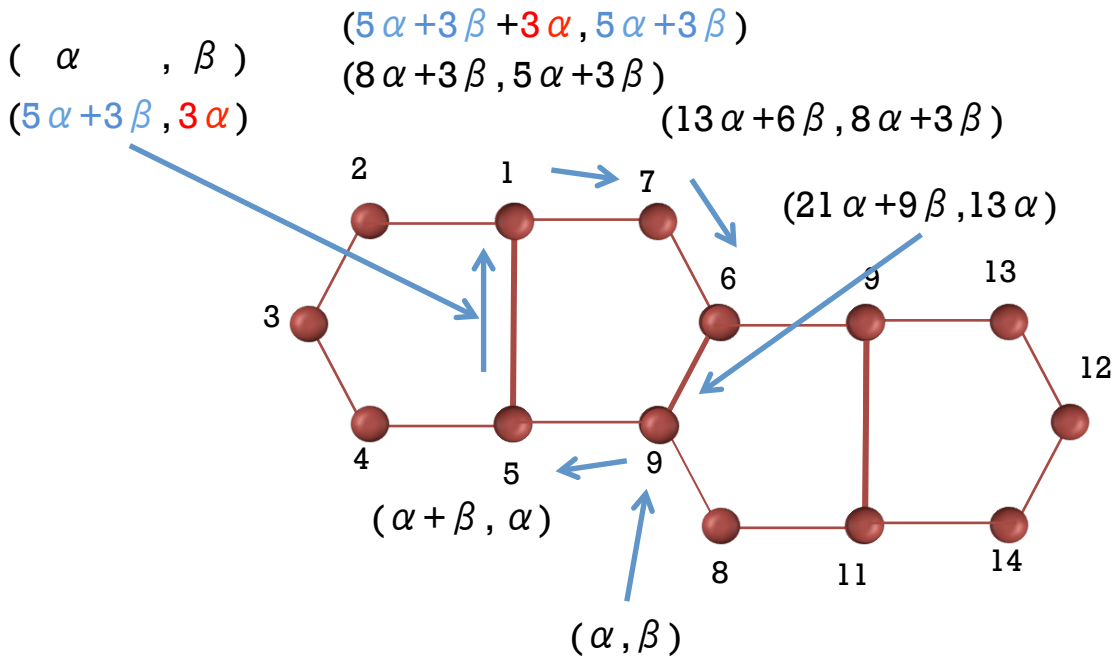

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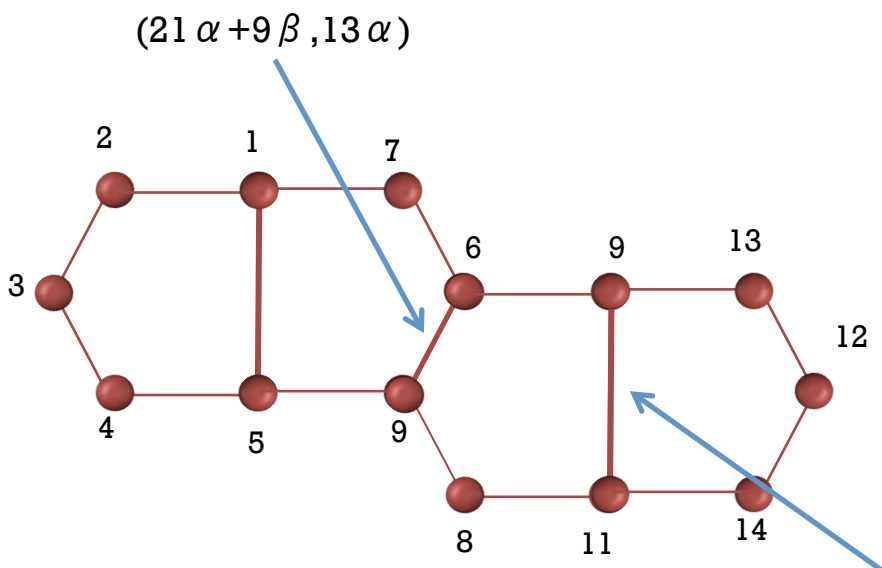

11) (α , β)
8) ($\alpha+\beta$, α)
9) ($2\alpha+\beta$, $\alpha+\beta$)
(2(21 α +9 β)+(13 α),
21 α +9 β +13 α)
6) (55 α +18 β ,34 α +15 β)
9) (89 α +33 β , 55 α +24 β)

(89 α +33 β , 55 α)

The Merrifield-Simmons index of *Pentalene*

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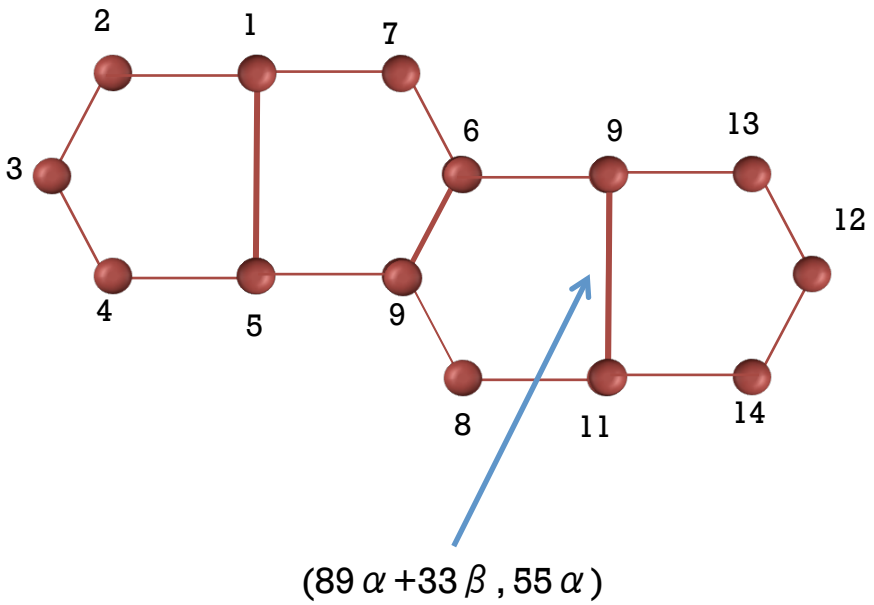
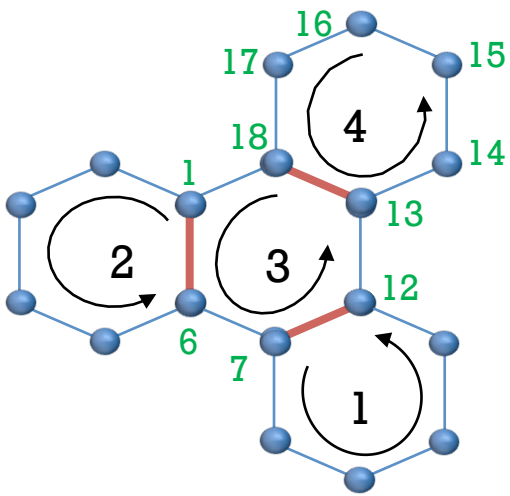


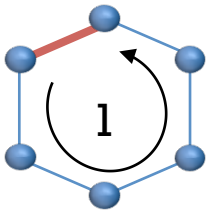
12) (α, β)
14) $(\alpha+\beta, \alpha)$
11) $(2\alpha+\beta, \alpha+\beta)$
$(2(89\alpha+33\beta)+(55\alpha),$
$89\alpha+33\beta+55\alpha)$
9) $(322\alpha+99\beta, 144\alpha+33\beta)$
13) $(466\alpha+132\beta, 322\alpha+99\beta)$

***NI(Pl)* = $(788\alpha+231\beta+466\alpha)$**

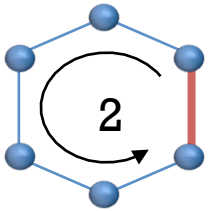
The Merrifield-Simmons index of Triphenylene

- Is a flat polycyclic aromatic hydrocarbon (PAH) consisting of four fused benzene rings.

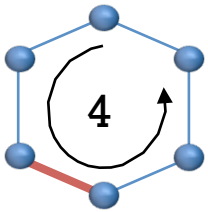




$(8\alpha + 5\beta, 5\alpha)$

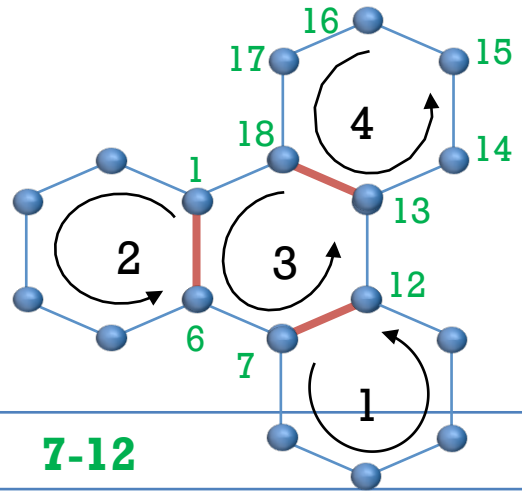


$(8\alpha + 5\beta, 5\alpha)$



$(8\alpha + 5\beta, 5\alpha)$

The Merrifield-Simmons index of Triphenylene



18	1-6	7	7-12	13

$(\alpha, \beta) \rightarrow (\alpha + \beta, \alpha)$

$\rightarrow 8(\alpha+\beta)+5(\alpha),5(\alpha+\beta)$

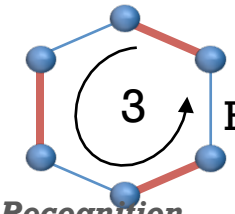
$\rightarrow (13\alpha+8\beta),5\alpha+5\beta)$

$\rightarrow (18\alpha+13\beta, 13\alpha+8\beta)$

$\rightarrow 8(18\alpha+13\beta)+5(13\alpha+8\beta),5(18\alpha+13\beta)$

$\rightarrow (209\alpha+144\beta, 90\alpha+65\beta)$

$\rightarrow (299\alpha+209\beta, 209\alpha+\cancel{144\beta})$



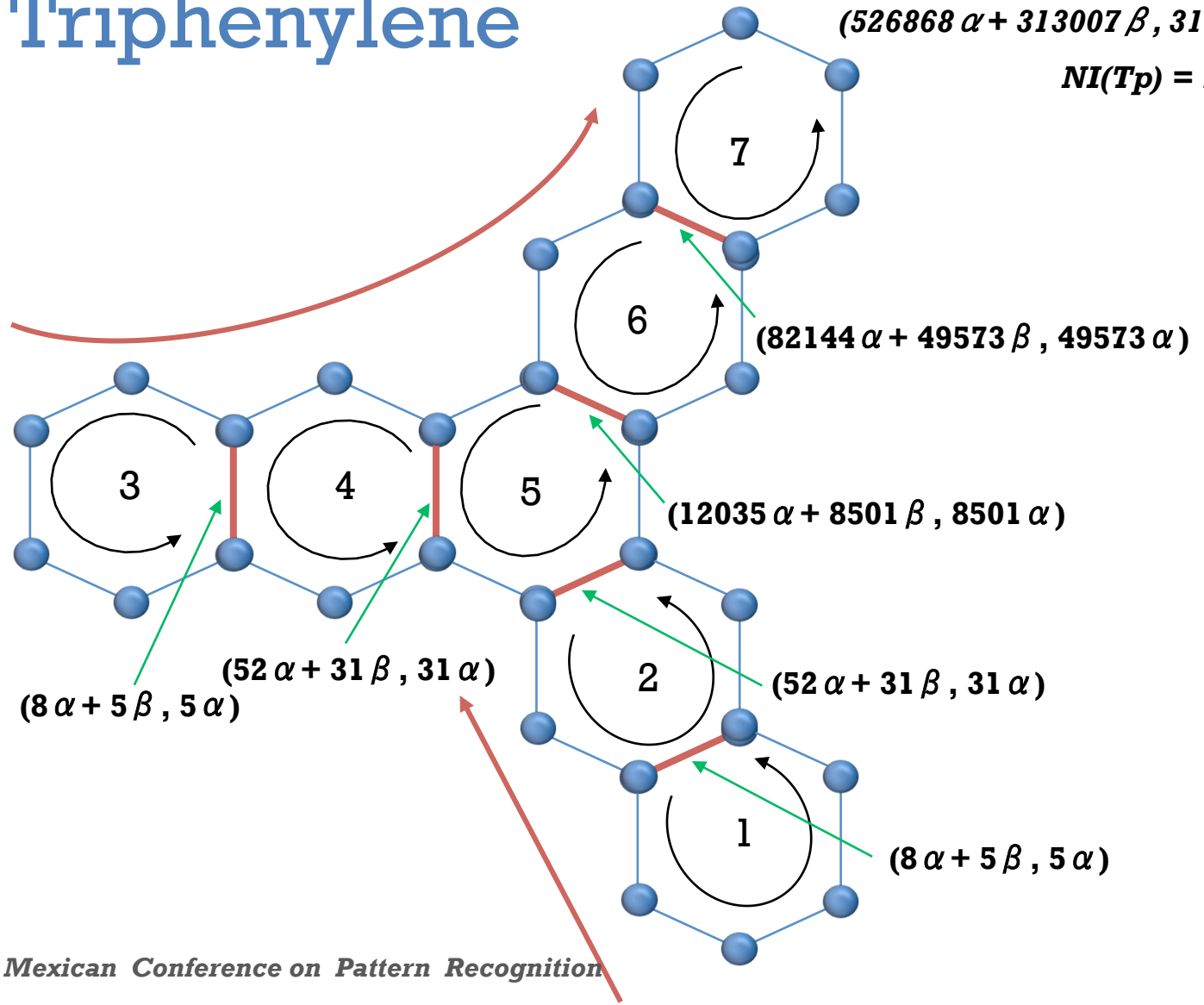
Hexagono 3 macro

$\rightarrow$ **$(299\alpha + 209\beta, 209\alpha)$**

The Merrifield-Simmons index of Triphenylene

$(526868\,\alpha + 313007\,\beta\,,\ 313007\,\alpha)$

$NI(Tp) = 1152882$



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Thanks for your attention.

Questions?