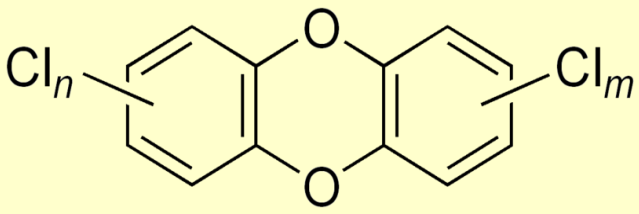
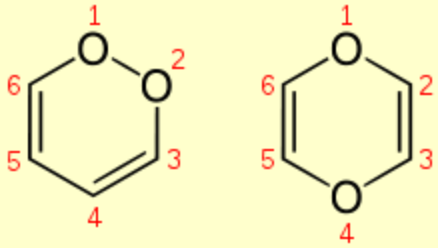


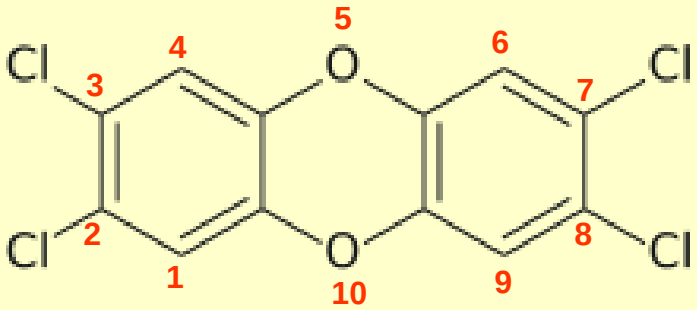
Polychlorinated dibenzodioxins

Dioxines
~200 stable compounds

toxic, when halogenated…



1,4-dioxin



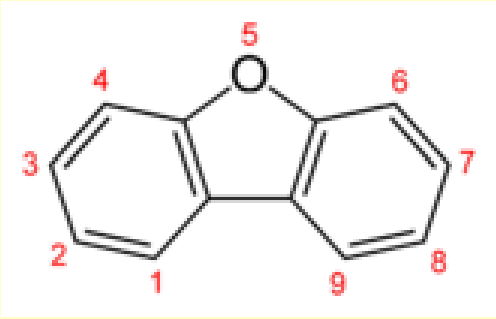
2,3,7,8-Tetrachlorodibenzo-*p*-dioxin (TCCD)

barely soluble in H_2O – highly in fat (x $10^{6)}$

TCDD (in man) half life 5 – 11 years

DL50 0.5 μg / Kg

di-benzofurans



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Healthy too…!!

Hypericin & Alzheimer d.

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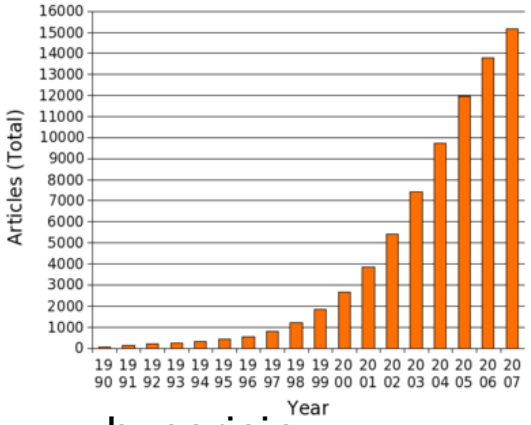
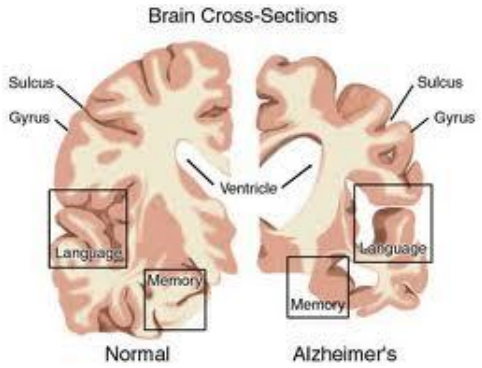
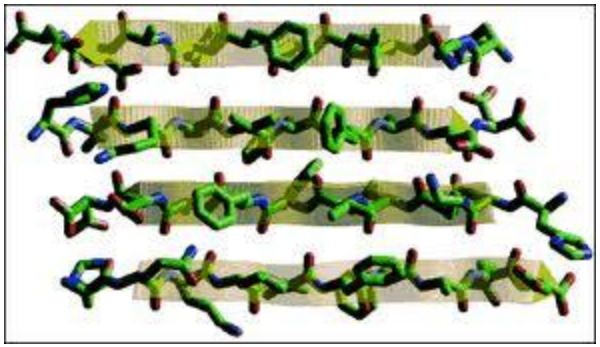
It perturbs β-amiloid polimerization processes
Read more: http://www.solaris.it/indexprima.asp?Articolo=1798#ixzz0Zgn7WMC9

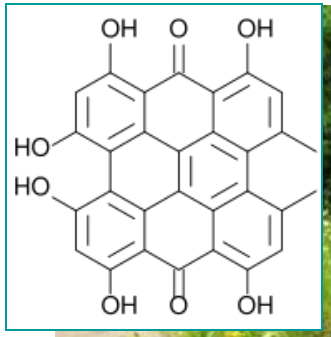


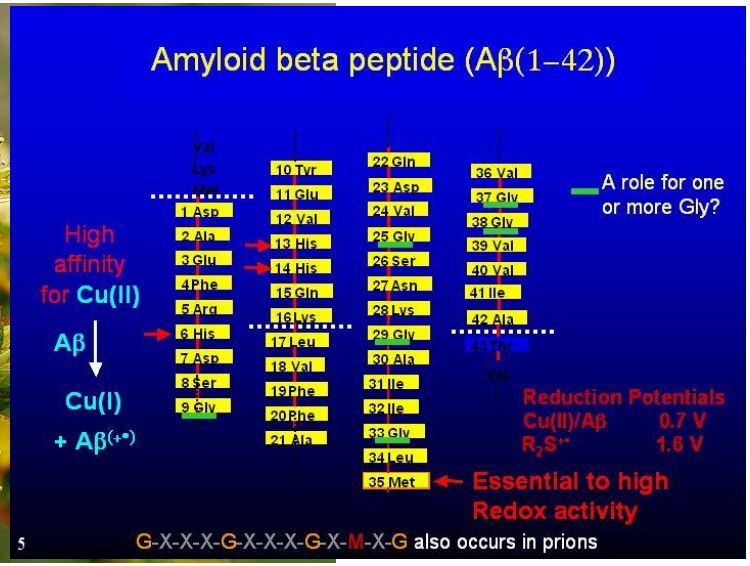


β-amiloid



hypericin





Ipericum (flower of S. Giovanni, *June 24th*)

Benzene, structure

$C_6H_6 + Cl_2 \longrightarrow C_6H_5\text{-}Cl + HCl$

***electrophilic substitution, i.e.* aromatic**

Halogenation (-Cl, -F, -Br)

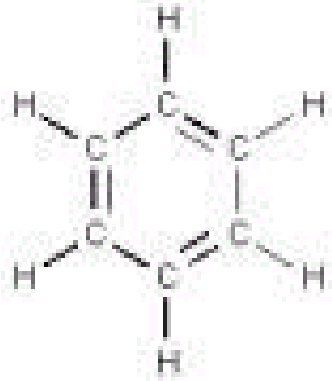
Nitration ($-NO_2$)

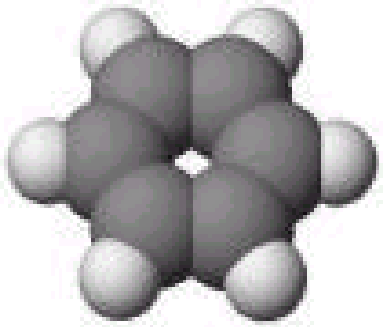
Sulfonation($-SO_3H$)

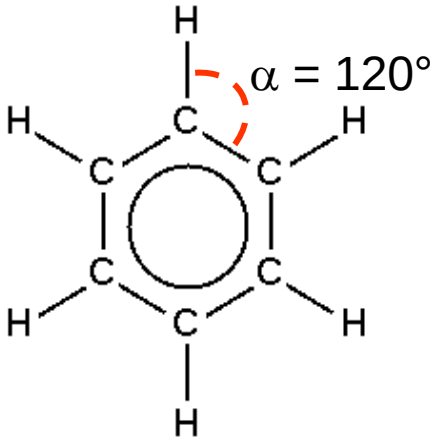
Acylation (-R)

Planar Structure

sp2 C
Exagonal (regular) → $\alpha = 120°$
Bond length 1,39 Å [single bond 1,54 Å - double bond 1,34Å]







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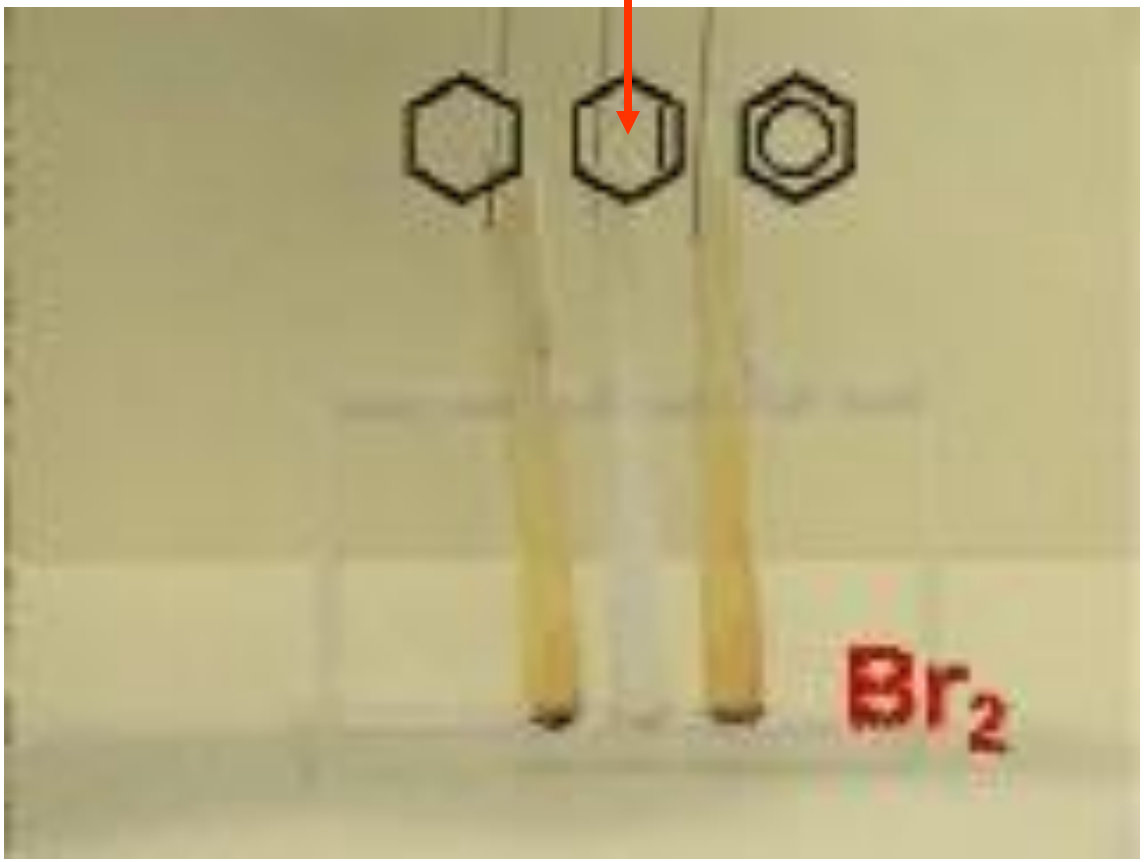
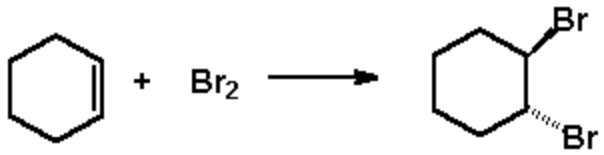


$C_6H_{10} + Br_2 \longrightarrow C_6H_{10}Br_2$



Cyclohexene (coloured) Colourless

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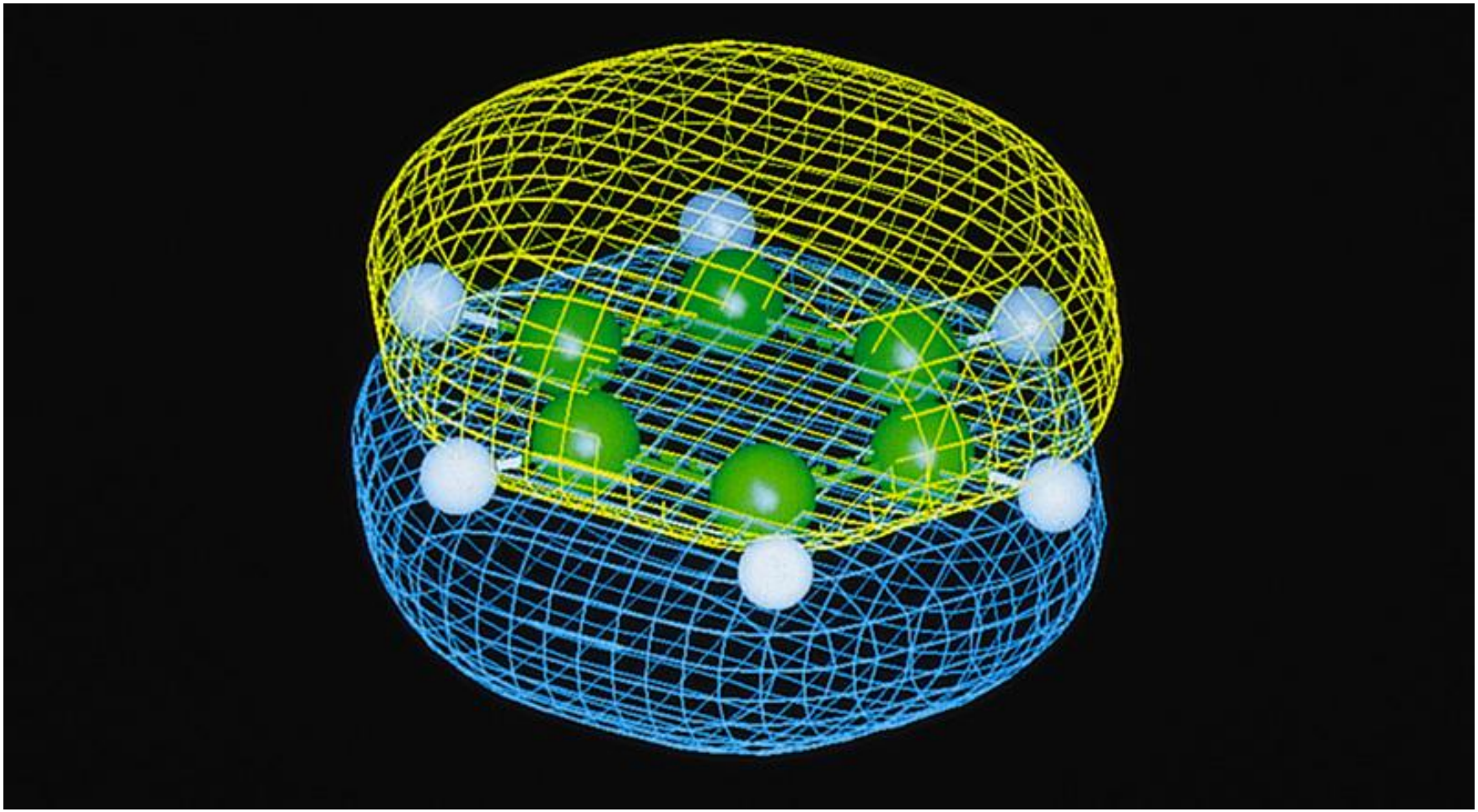
Cyclohexene reacts with bromine to give a colourless product but **cyclohexane and benzene do not**.

What is giving energy to force the ring on a single plane ?
p electrons, delocalized in π- system



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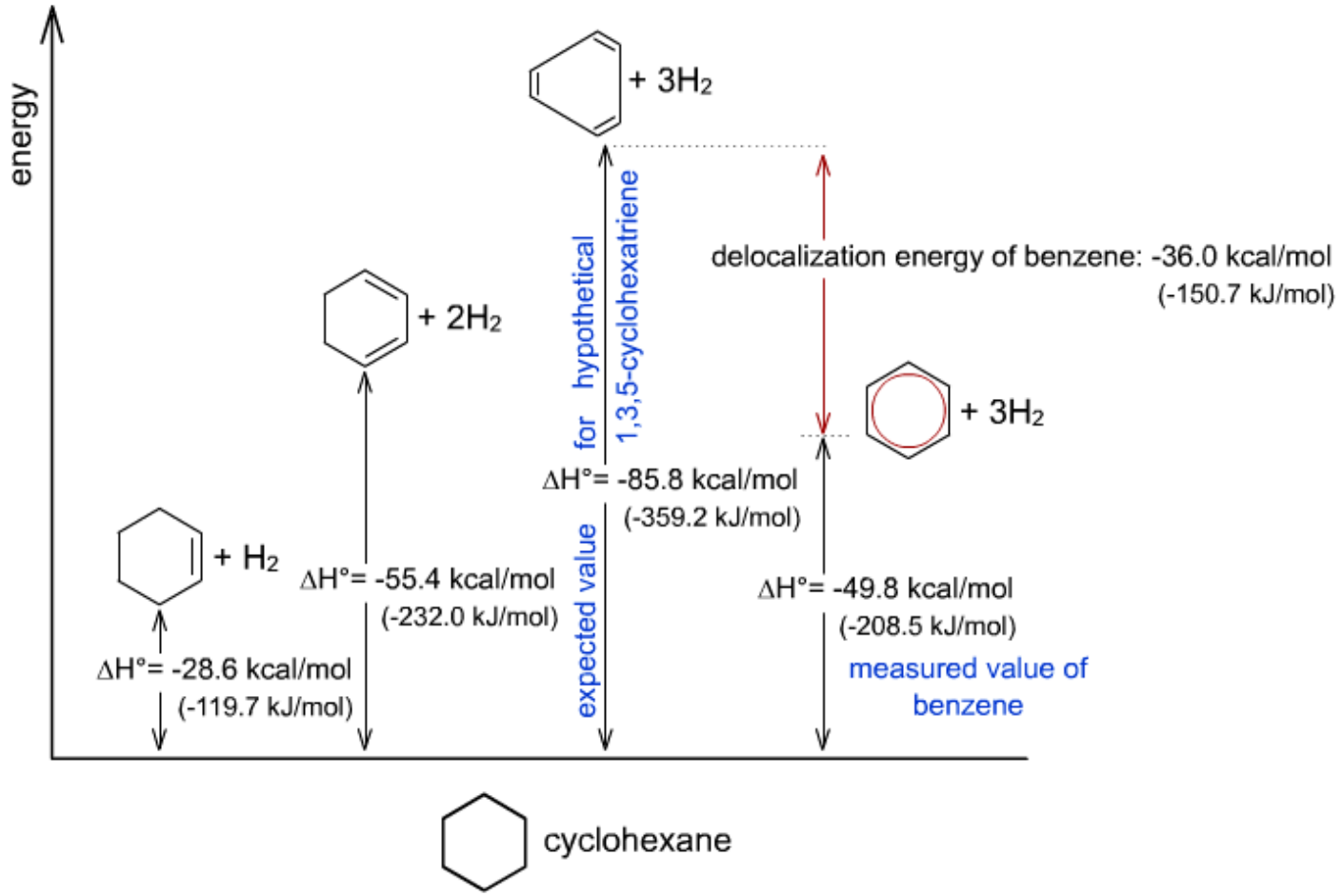
Aromatic energy



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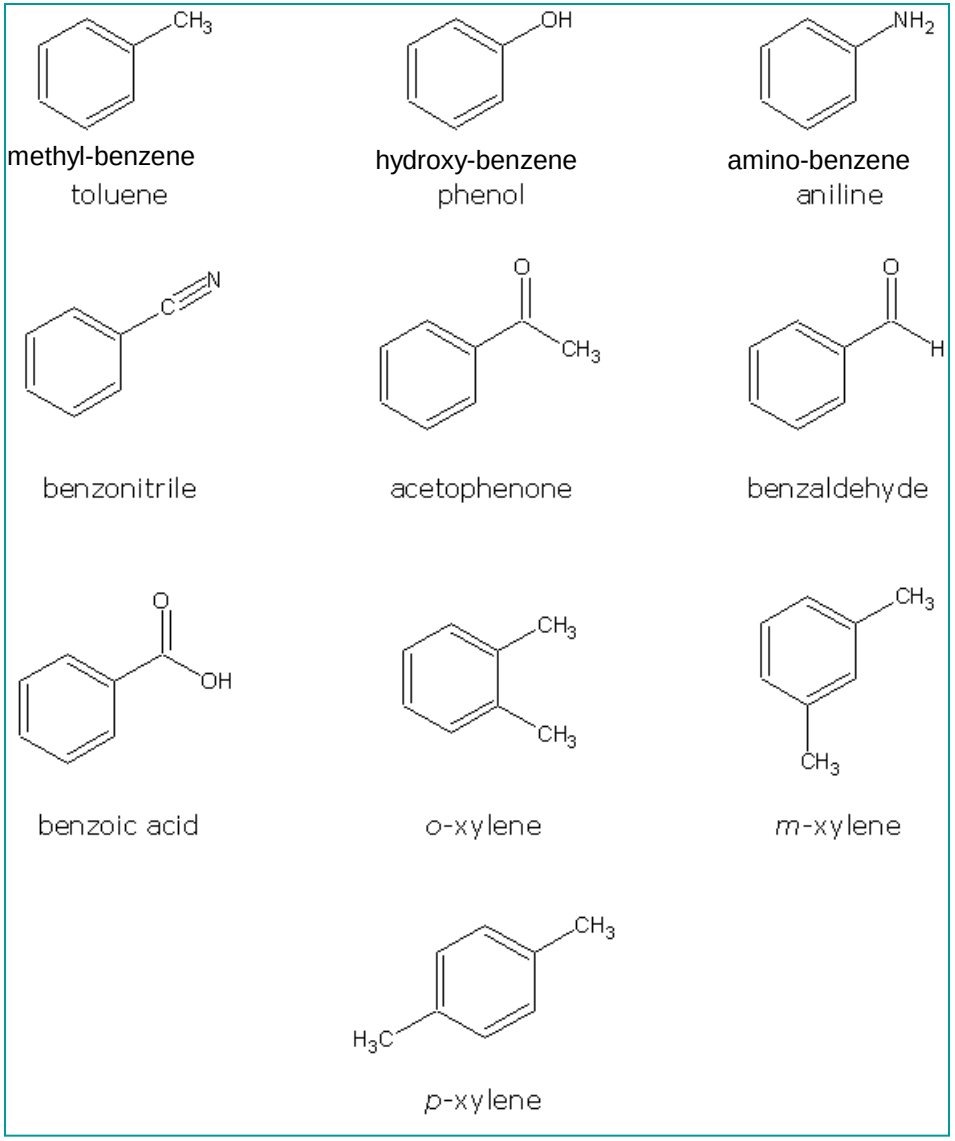
Nomenclature
Common definitions & IUPAC



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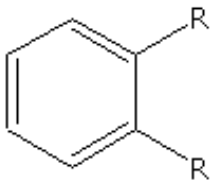
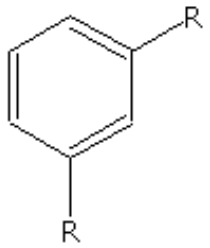
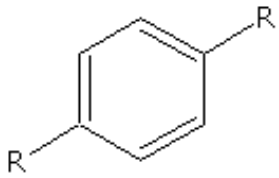
Di-substituted benzene derivatives



ortho

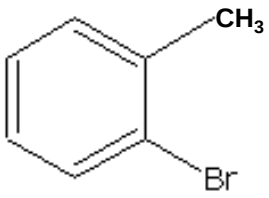


meta

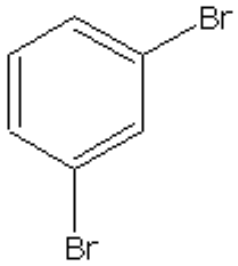


para

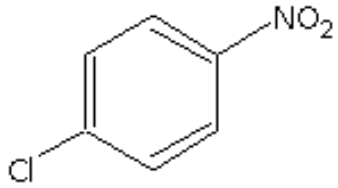
Examples:



ortho-bromotoluene



meta-dibromobenzene



para-chloronitrobenzene

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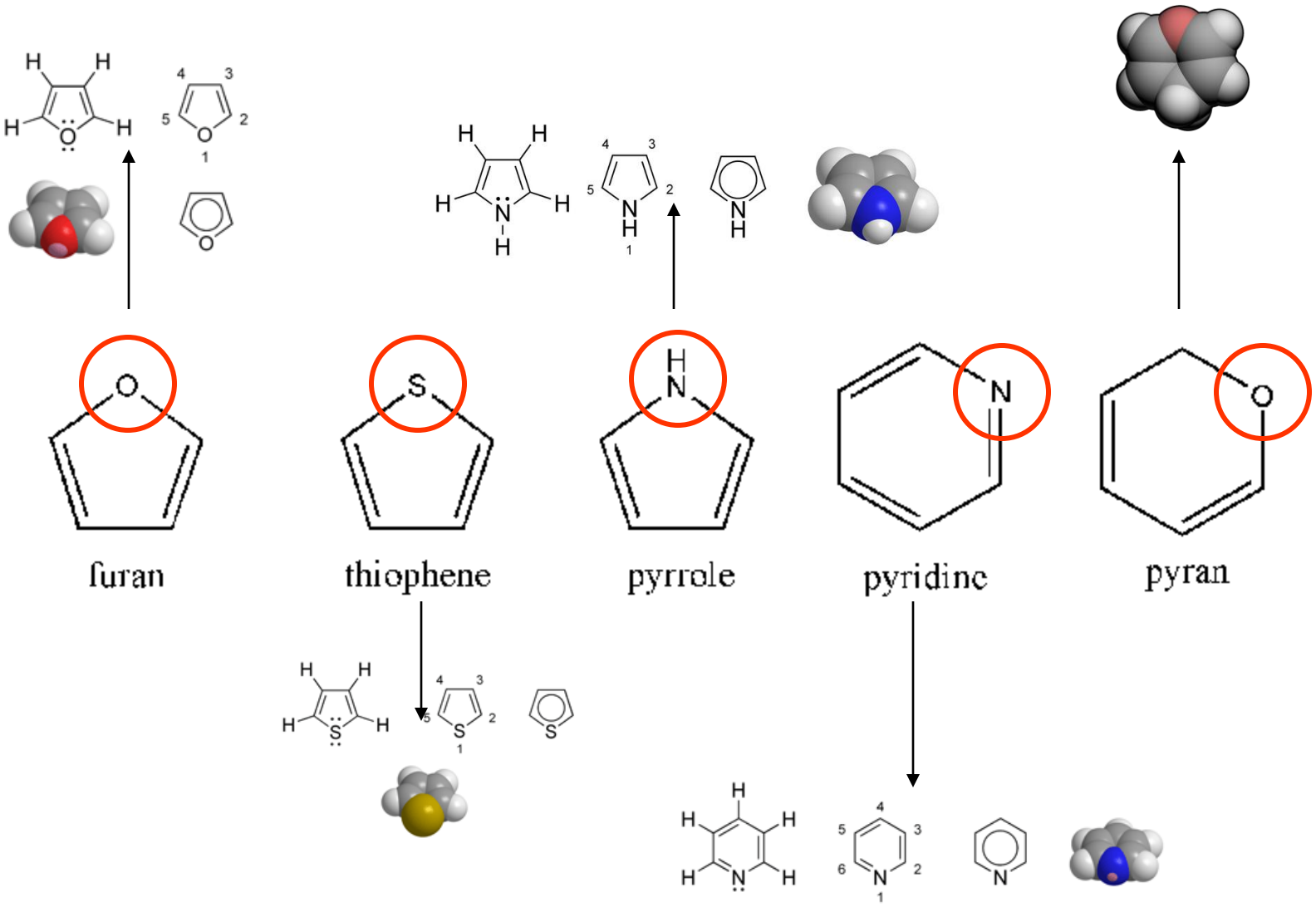
Heterocyclic compounds: ring including (at least) 1 heteroatom (N,S,O *etc*.)



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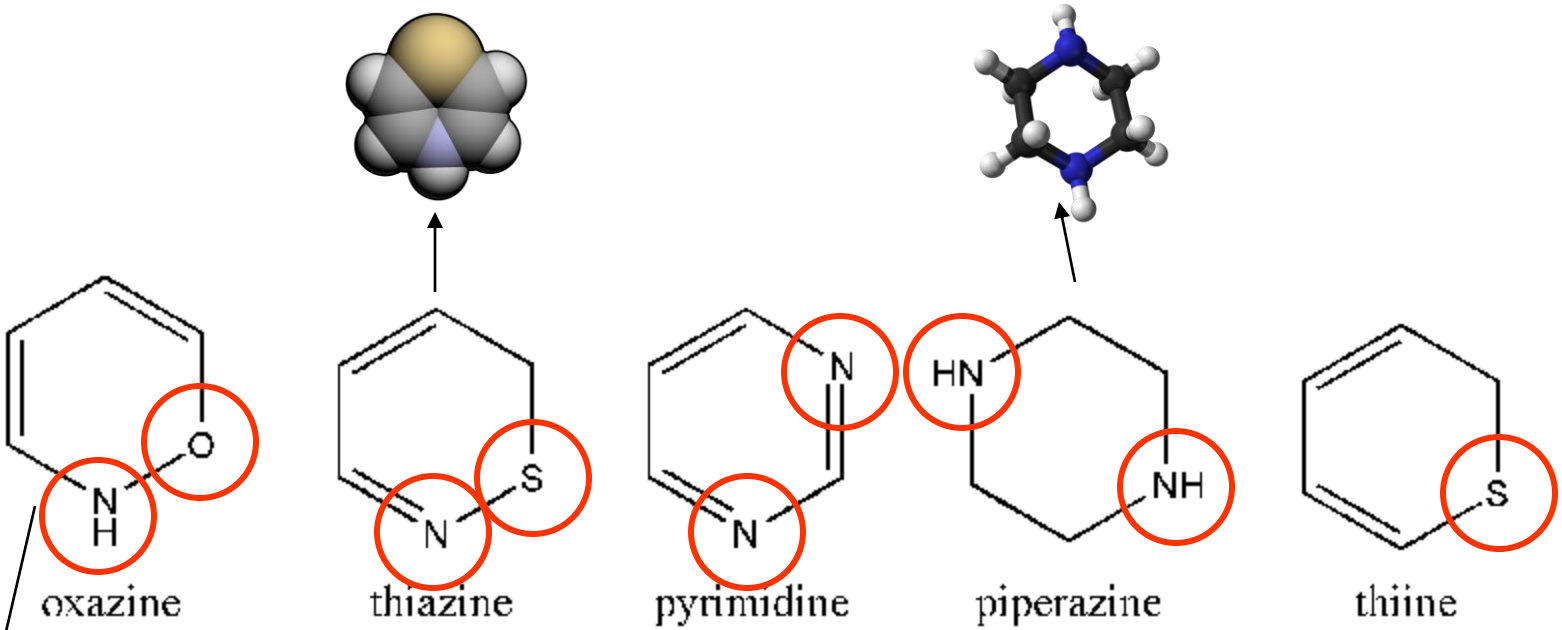
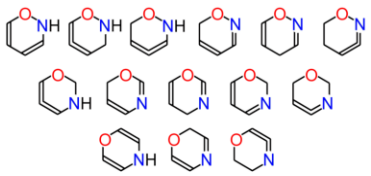
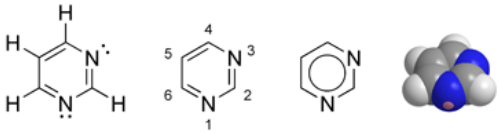
Heterocyclic compounds: ring including 2 heteroatoms (N,S,O *etc*.)





Photocromic polymers



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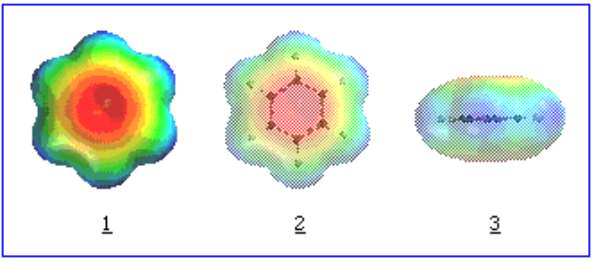
Hückle (*von Doering*) rule

For a ring to be aromatic,
the number of π electrons
should be 4n + 2 elettroni *p* delocalizzati
in un sistema di risonanza.
(Es. n = 1, 2, 3 *etc*.)

carbocyclic

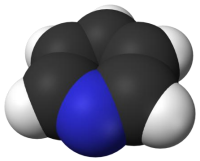
Benzene (n =1)



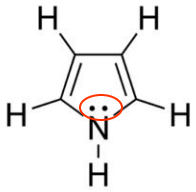
heterocyclic

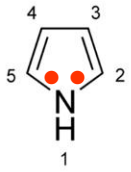
$_7N = 1s^2\ 2s^2\ 2p^3$

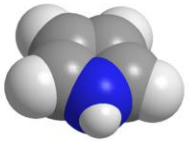
Pyridine
N →1 e- π



Pyrrole
N → 2 e- π







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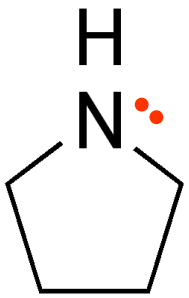
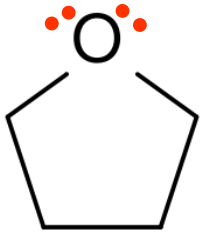
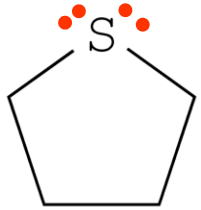
Heterocyclic - alyphatics



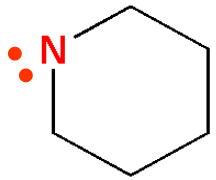
pyrrolidine, sp3



tetra-hydrofuran, sp3

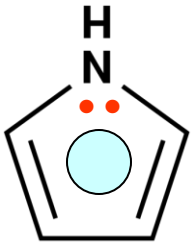


tetra-hydrothiophene, sp3

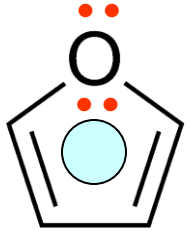


piperidine, sp3

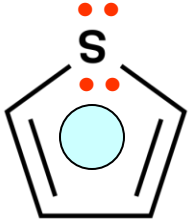
Heterocyclic - aromatics



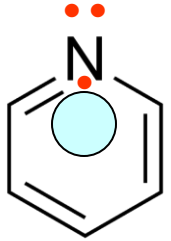
pyrrole, sp2



furan, sp2



thiophene, sp2



pyridine, sp2

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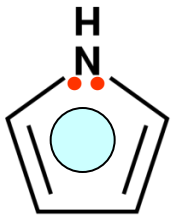
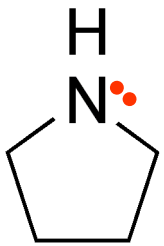
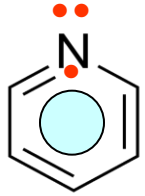
Basic properties of the N-heterocyclic compounds



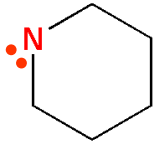
pyrrole, Kb = 4×10^{-19}



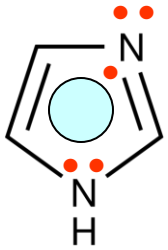
pyrrolidine, Kb = 1.3×10^{-3}
1 lone pair, sp3



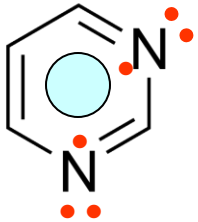
pyridine, Kb = 2.3×10^{-9}
1 lone pair, sp2



piperidine, Kb = 1.6×10^{-3}
1 lone pair, sp3



imidazole, Kb 1.2×10^{-7}
1 lone pair, sp2



pyrimidine, Kb_1 1.7×10^{-13}
2 lone pairs, sp2

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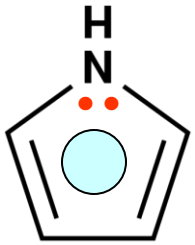
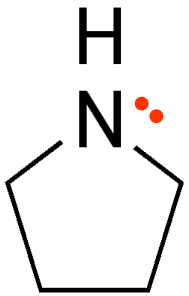
Heterocyclic derivatives

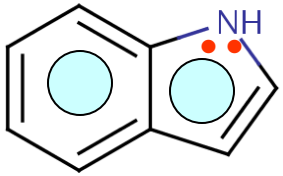
Penta-derivatives, 1 N atom



pyrrole

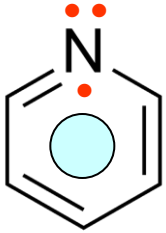


pyrrolidine

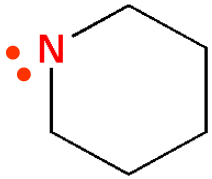


indole

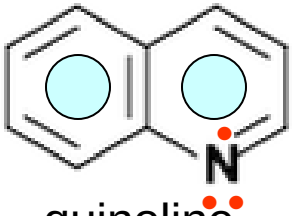
Hexa-derivatives, 1 N atom



pyridine



piperidine



quinoline

quinine
strychnine
papaverine

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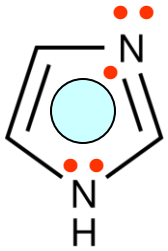
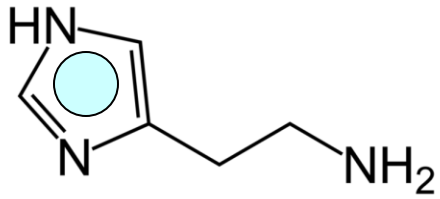
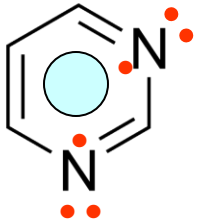
Hetrocyclic derivatives – 2 N



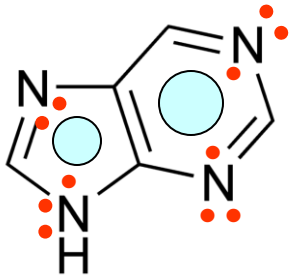
imidazole



histamine



pyrimidine



purine

DNA, RNA bases
pyrimidines : thymine, cytosine, uracil
purines: adenine, guanine

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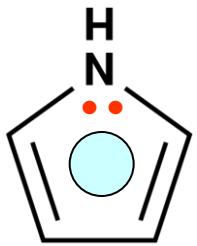
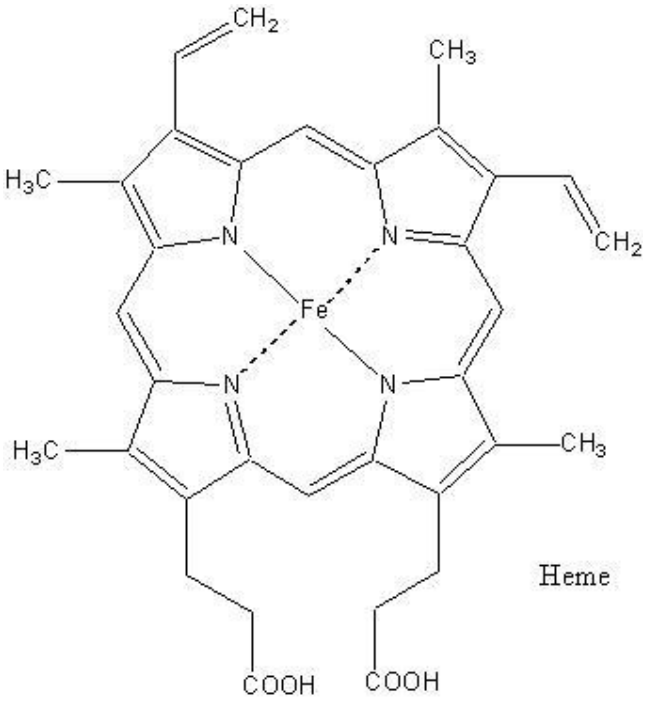
Pyrrole - derivatives





Heme

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Aromatic molecules
Can be particularly dangerous
“planar rings…” !

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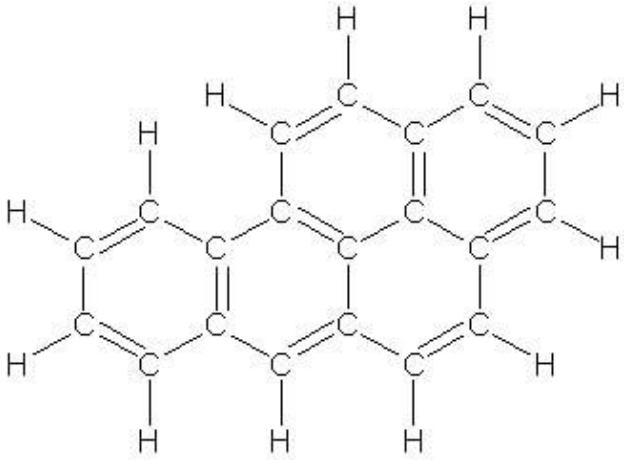
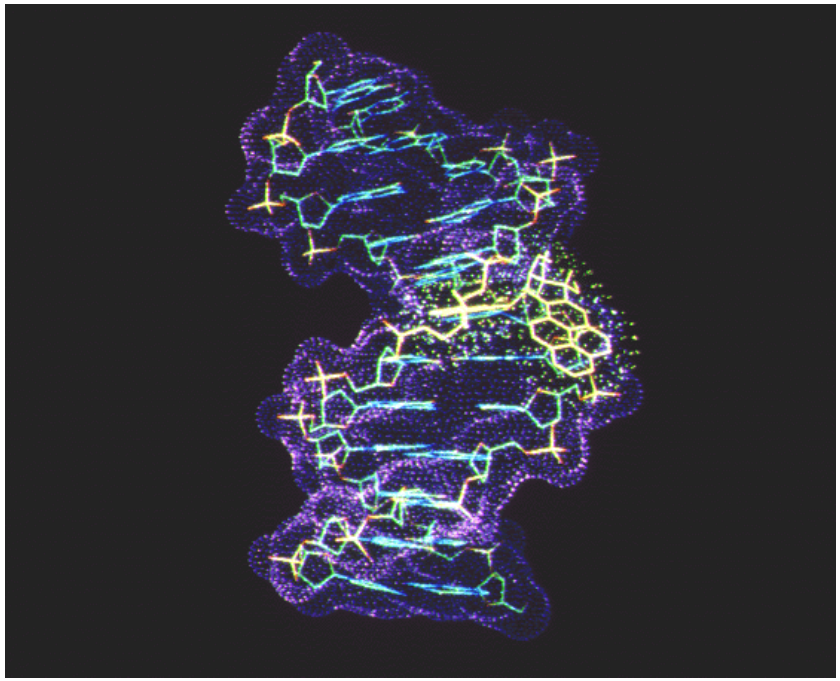


The benzopyrene
&
The DNA-*gatekeeper*



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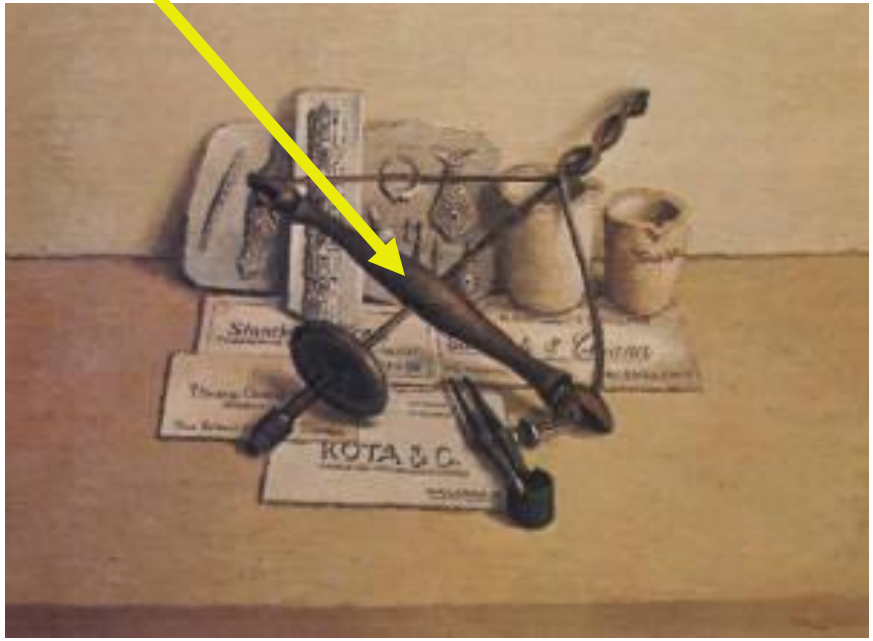
gatekeeper



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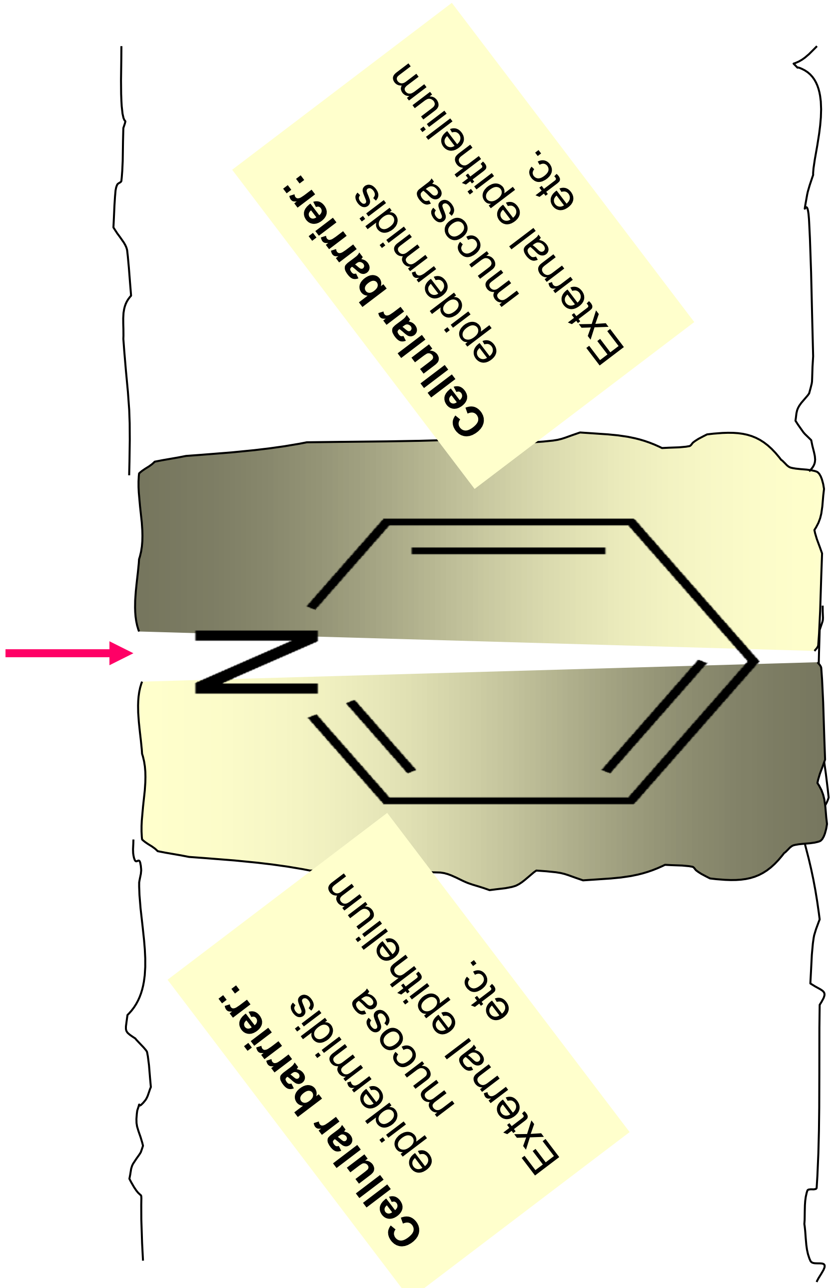
inter
H_2O, hydrosoluble compounds



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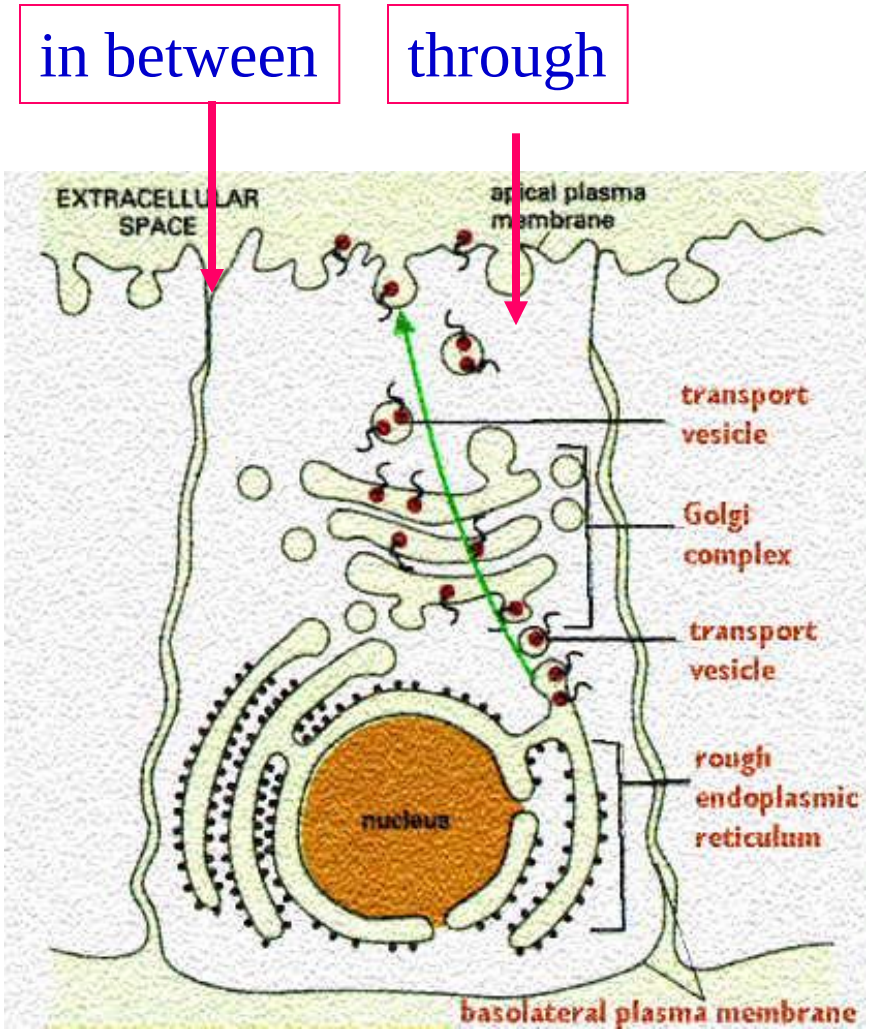
External chemical agent penetration



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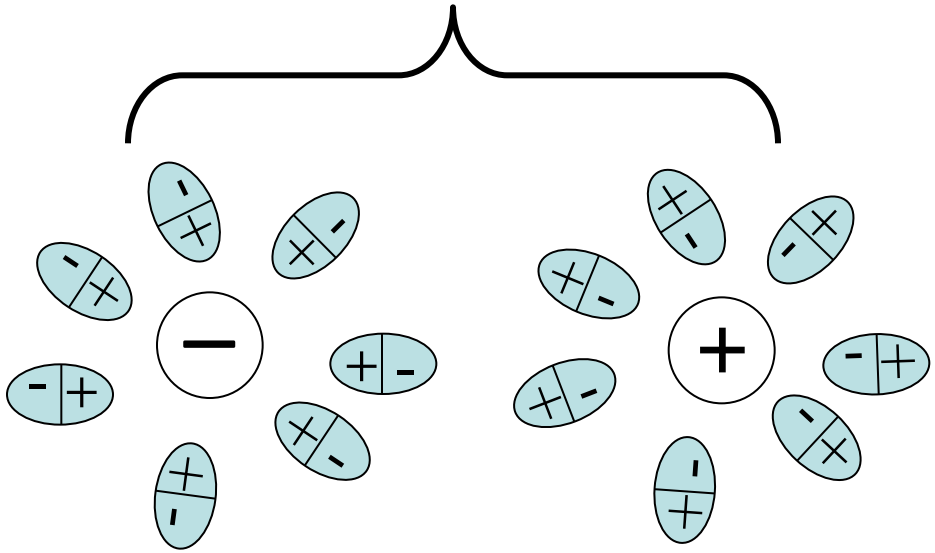
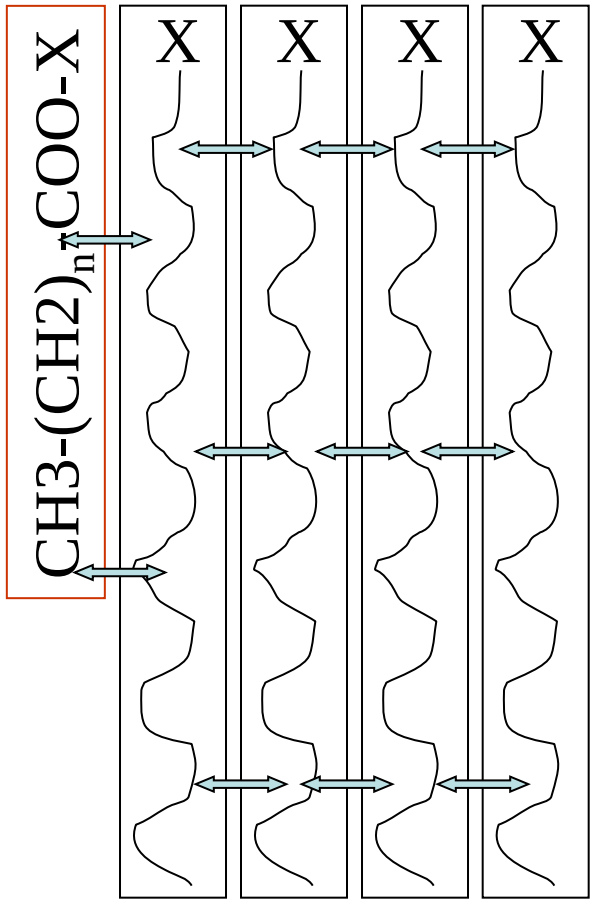
Hydrophilic interactions



Charge mediated

Hydrophobic interactions



London Van der Waals mediated

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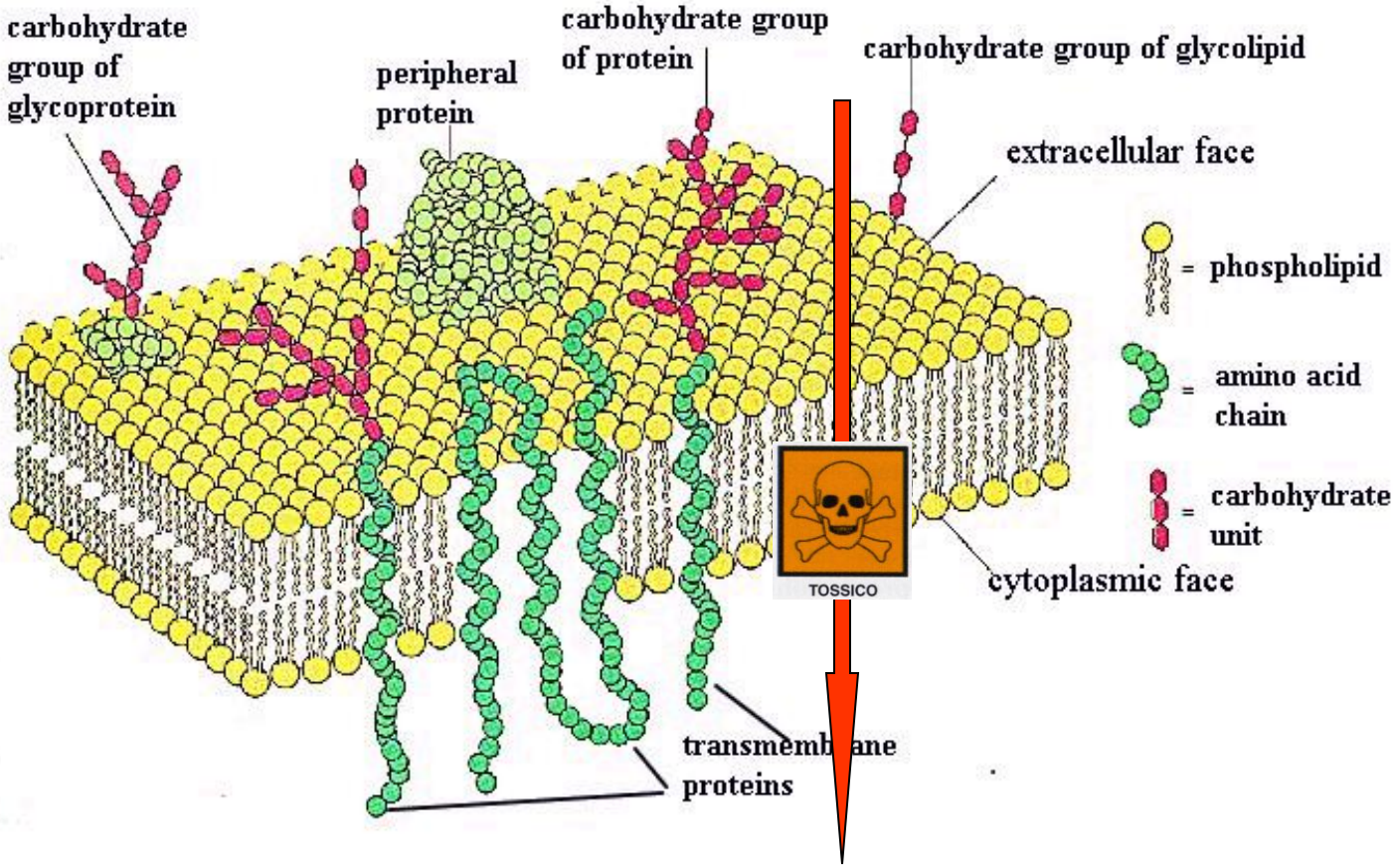
Schematic drawing



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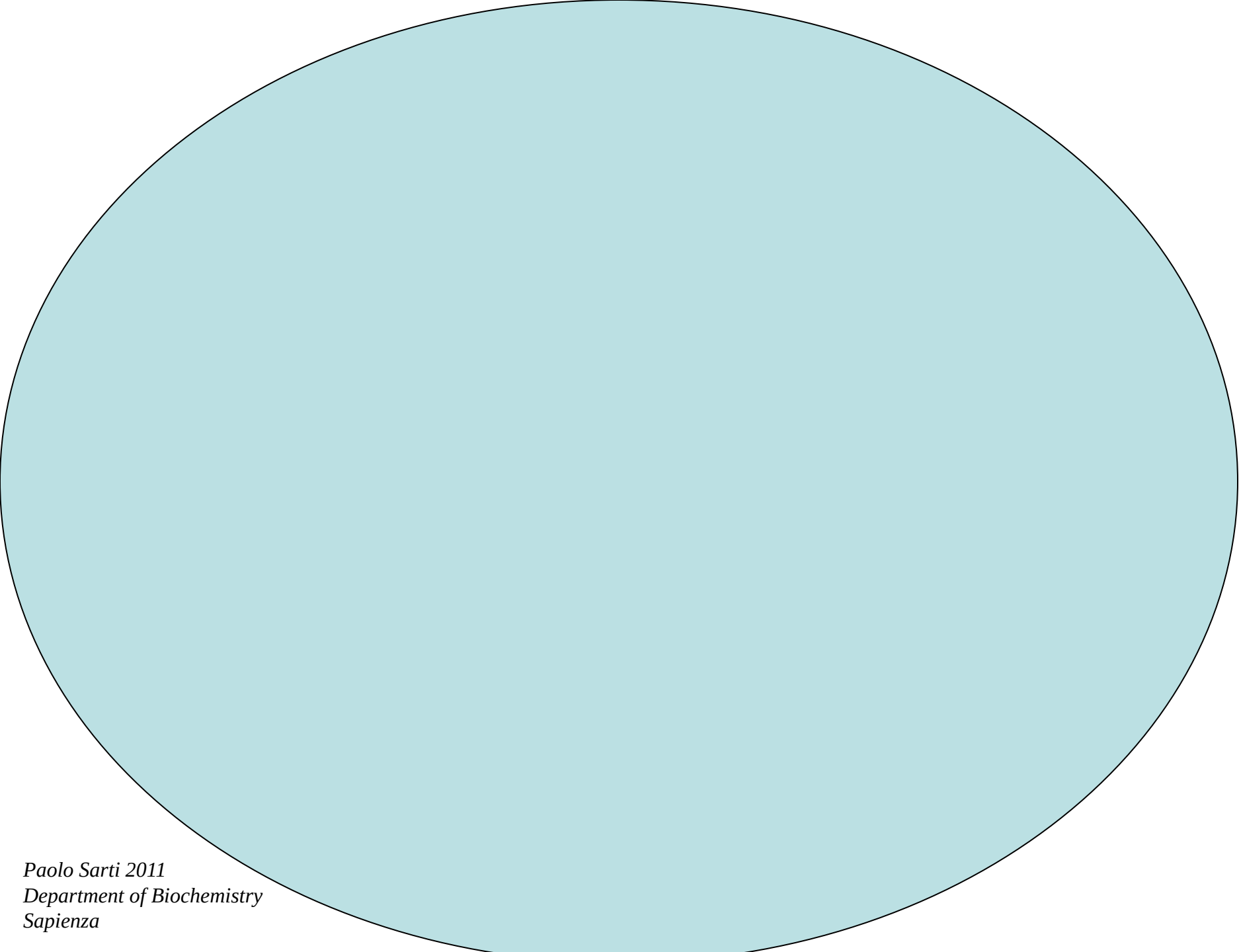

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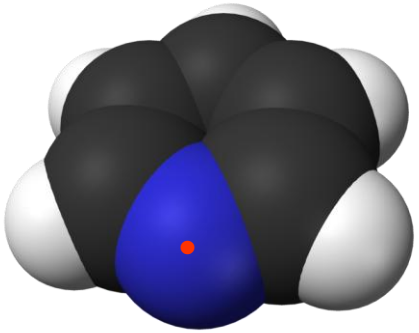
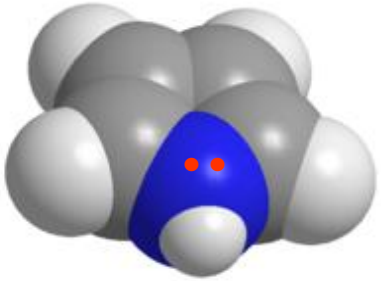
N-hybridization (sp2)

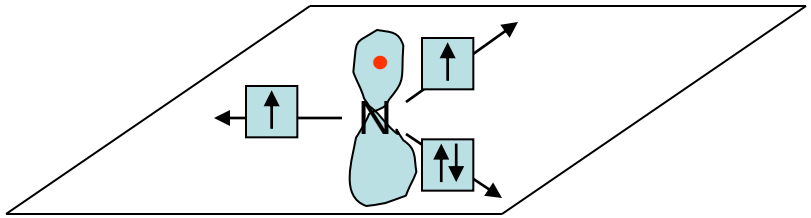
pyridine

pyrrole

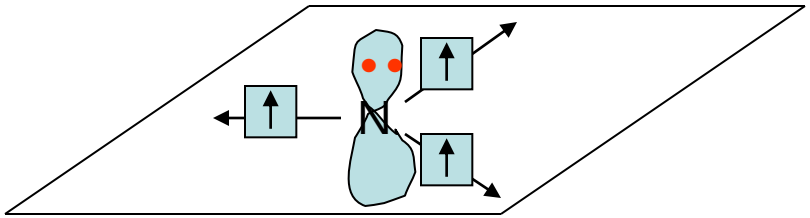


Huckel, 6 e- π ?





Sp2 plane



Sp2 plane

$_{7}N = 1s^2\ 2s^2\ 2p^3$

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