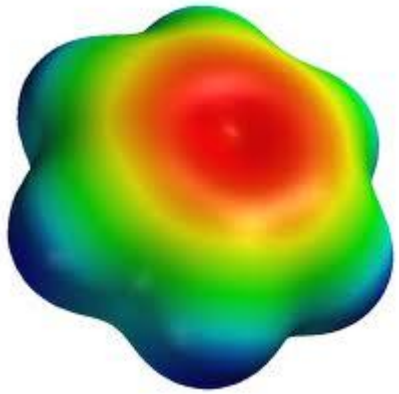
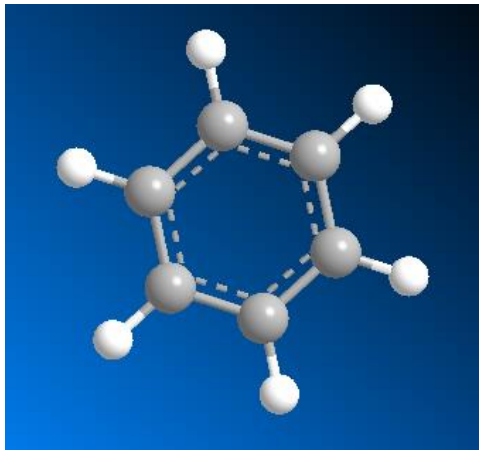
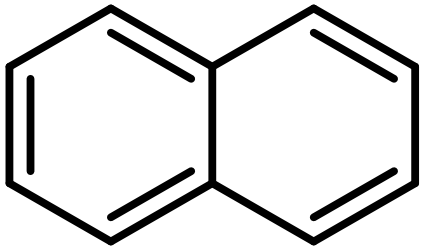


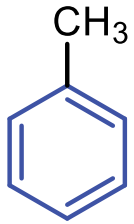


# Areny

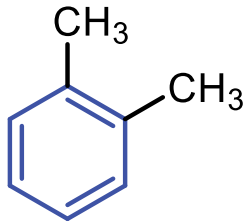



# Aromatické uhlovodíky získávané destilací ropy

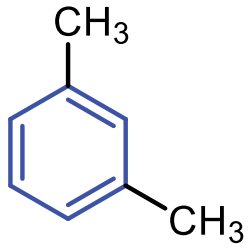
**Benzen**
**t.v. 80°C**



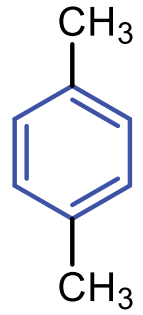

**Toluen**
**t.v. 111°C**



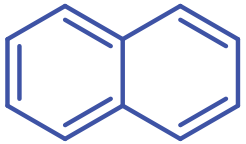

***o*-Xylen**
**t.v. 144°C**



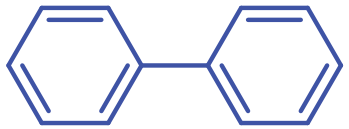

***m*-Xylen**
**t.v. 139°C**



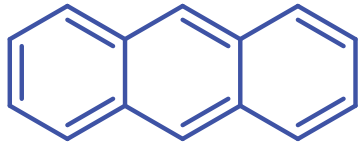

***p*-Xylen**
**t.v. 138°C**



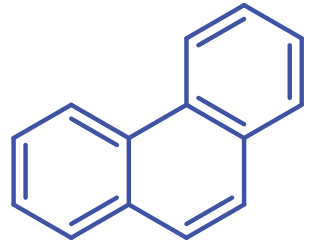
**Naftalen**
**t.t. 80°C**



**Bifenyl**
**t.t. 71°C**

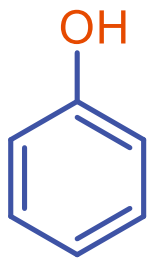


**Anthracen**
**t.t. 216°C**

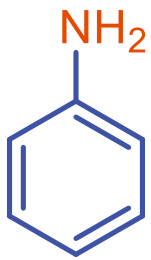


**Fenanthren**
**t.t. 101°C**

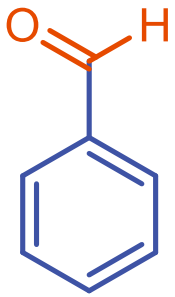
# Triviální názvy některých dalších důležitých derivátů benzenu



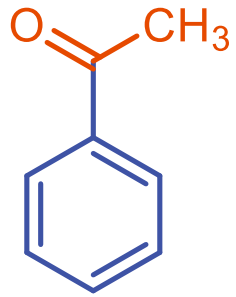

**Fenol**
**t.t. 43°C**



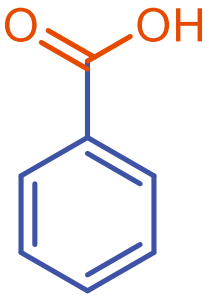

**Anilin**
**t.v. 184°C**



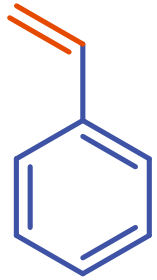

**Benzaldehyd**
**t.v. 178°C**




**Acetofenon**
**t.t. 21°C**



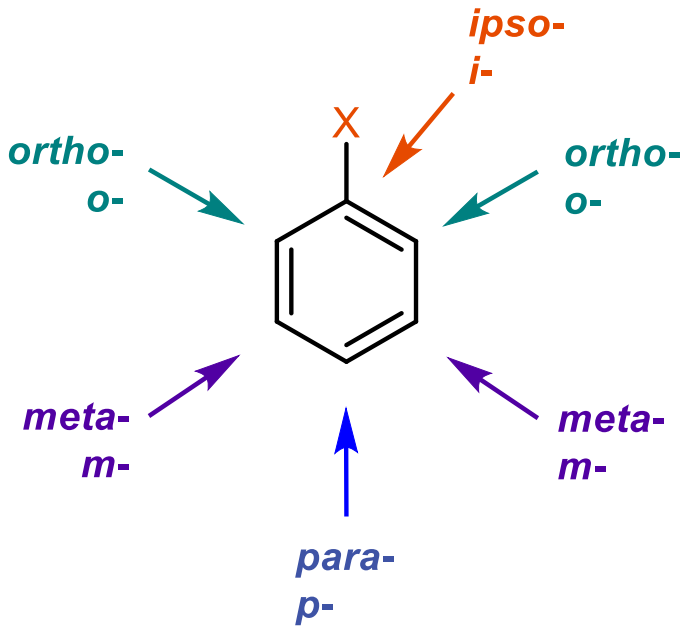

**Kyselina benzoová**
**t.v. 178°C**

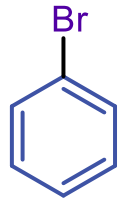


**Styren**
**t.v. 145°C**

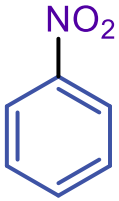
**Kumen**
**t.v. 152°C**

# Deriváty benzenu - názvosloví

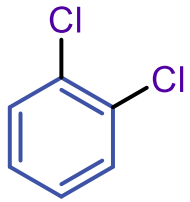


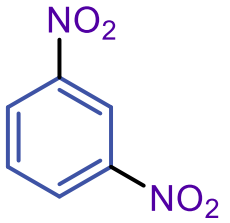

brombenzen



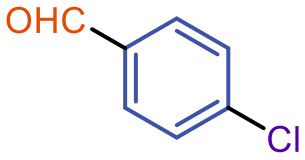

nitrobenzen



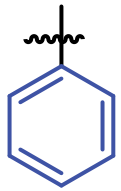

*o*-dichlorbenzen
*ortho*-dichlorbenzen
1,2-dichlorbenzen



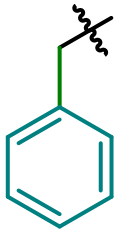

*m*-dinitrobenzen
*meta*-dinitrobenzen
1,3-dinitrobenzen



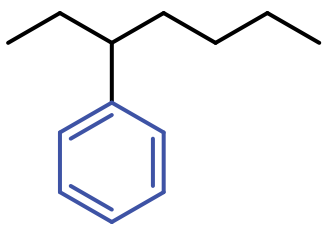

*p*-chlorbenzaldehyd
*para*-chlorbenzaldehyd
4-chlorbenzaldehyd



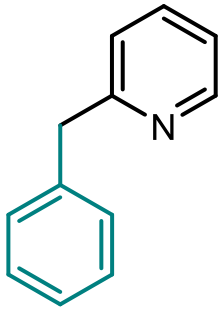
fenyl



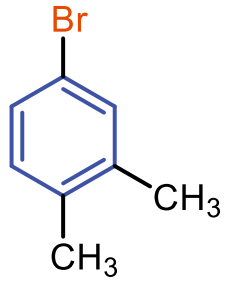
benzyl



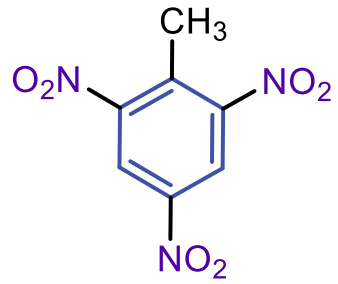
3-fenylheptan




2-benzylpyridin

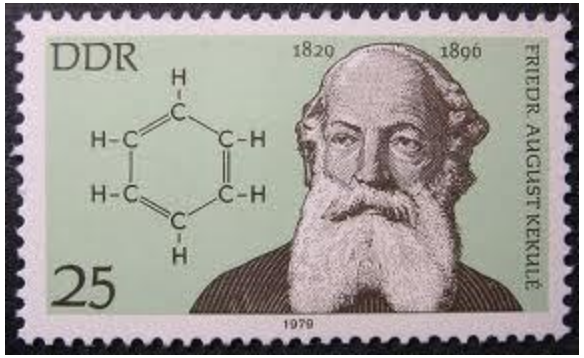



4-brom-1,2-dimethylbenzen



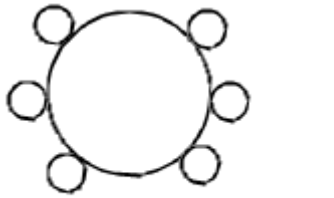

2,4,6-trinitrotoluen

# Struktura benzenu - historie

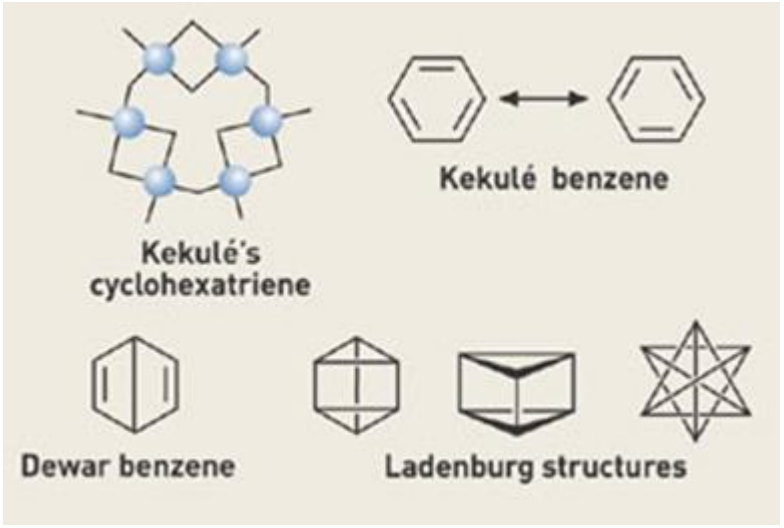




**1865**

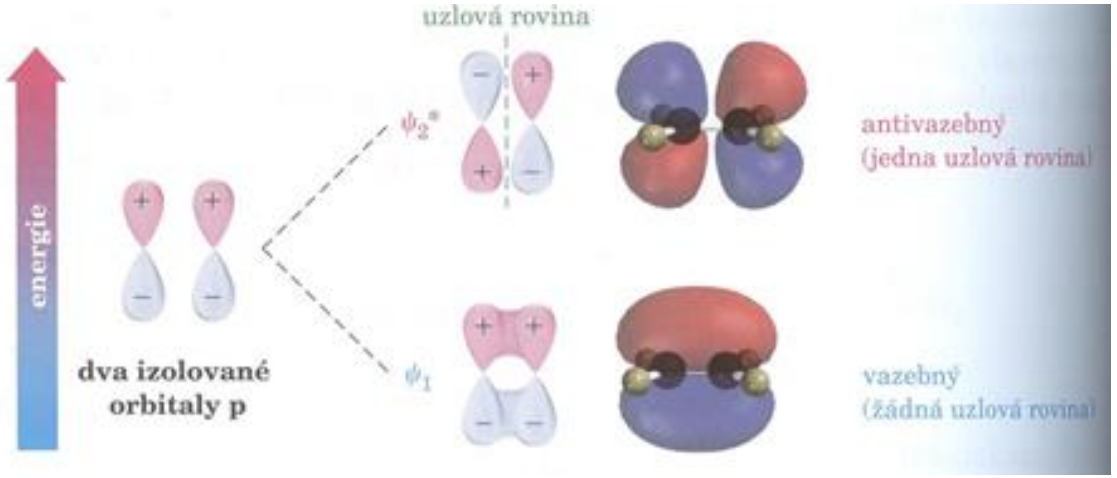
$C_6H_6$, symetrická molekula, neprobíhají adiční reakce



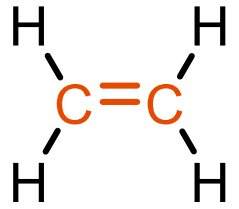
**Loschmidt 1861**



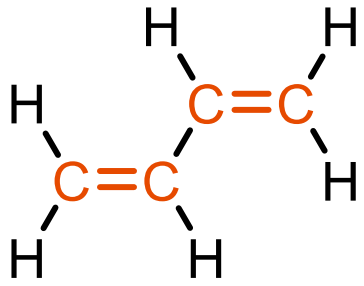
# Konjugované p-systémy a delokalizace elektronů

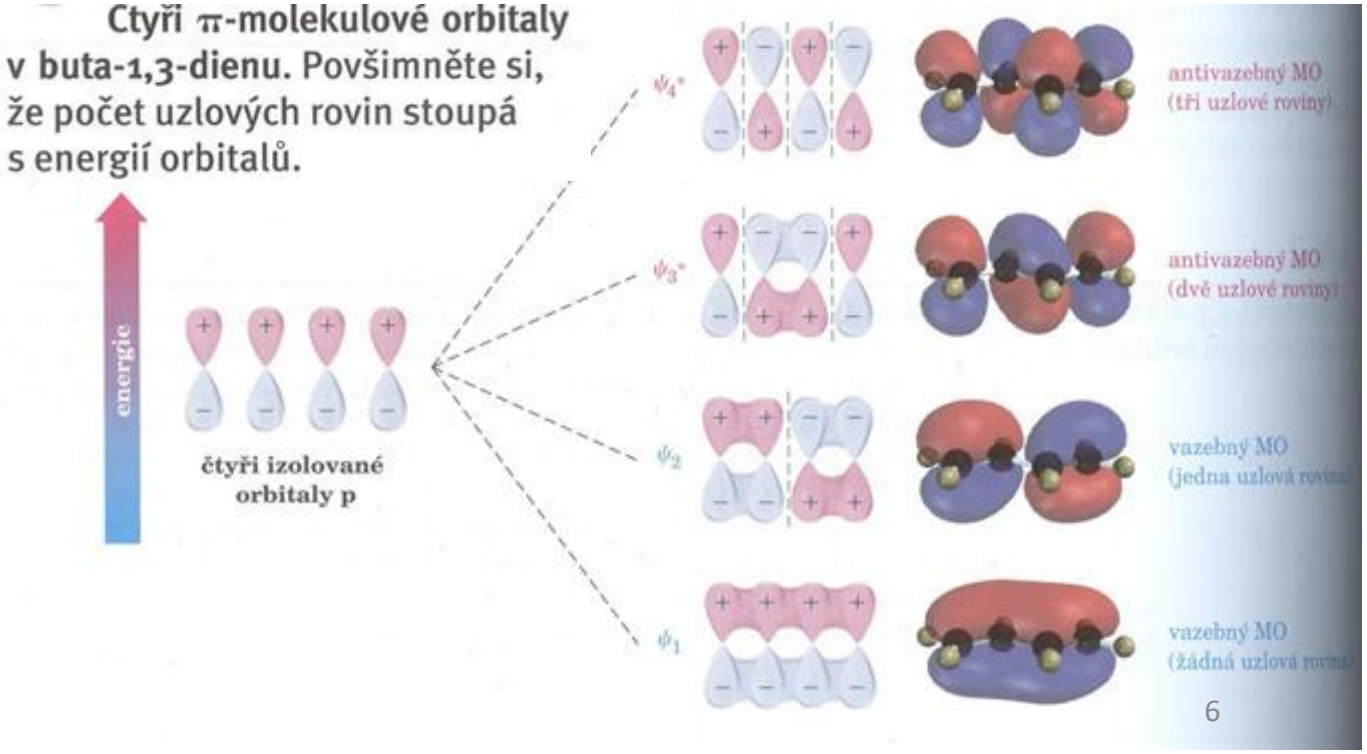


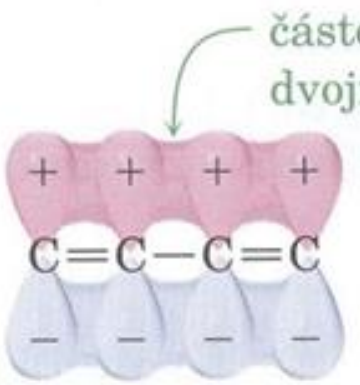

**Ethen** - izolovaná dvojná vazba



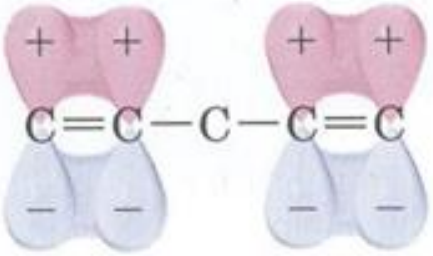

**Butadien** - konjugované dvojné vazby



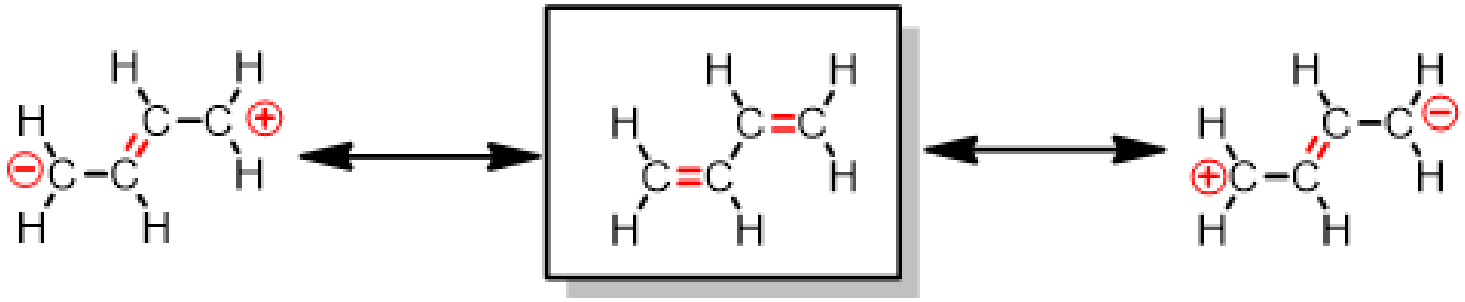



**buta-1,3-dien**
**konjugovaný dien**

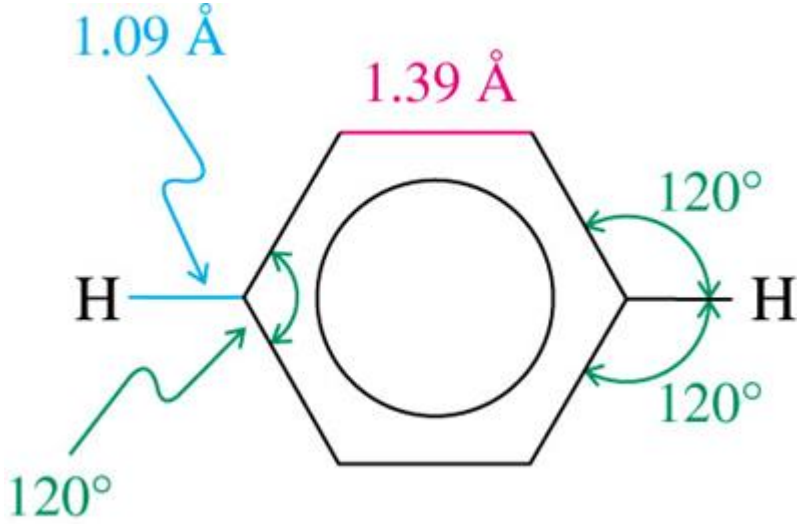


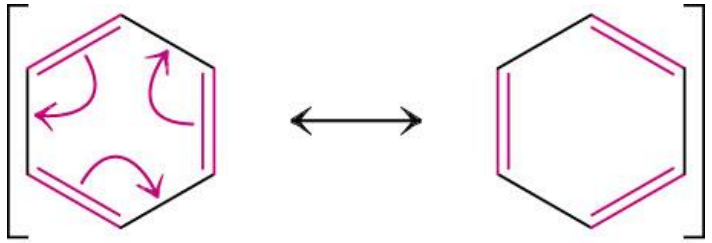

**penta-1,4 dien**
**nekonjugovaný dien**

**Dochází k částečné delokalizaci elektronů v rámci celého konjugovaného π-systému**

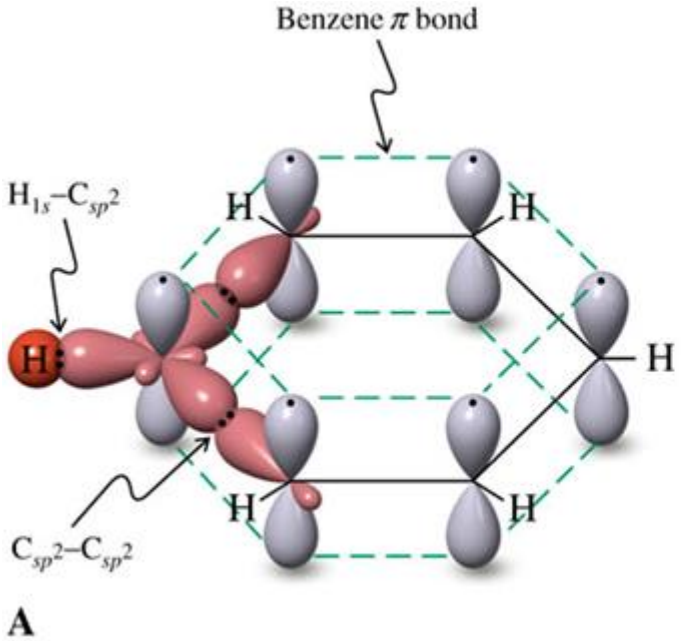


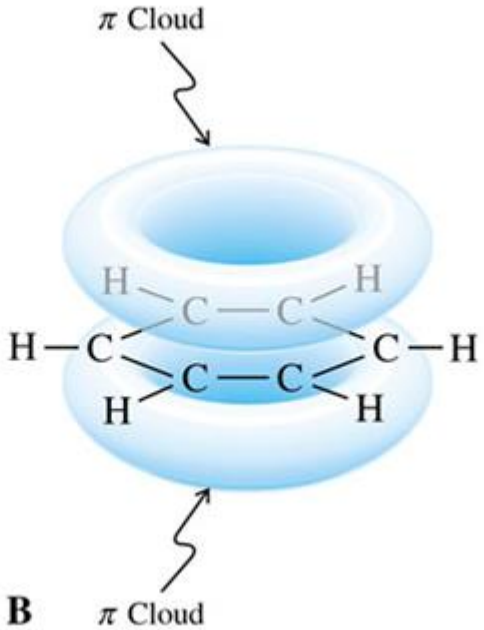
# Benzen

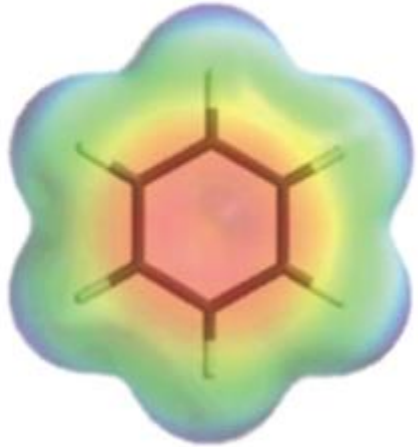


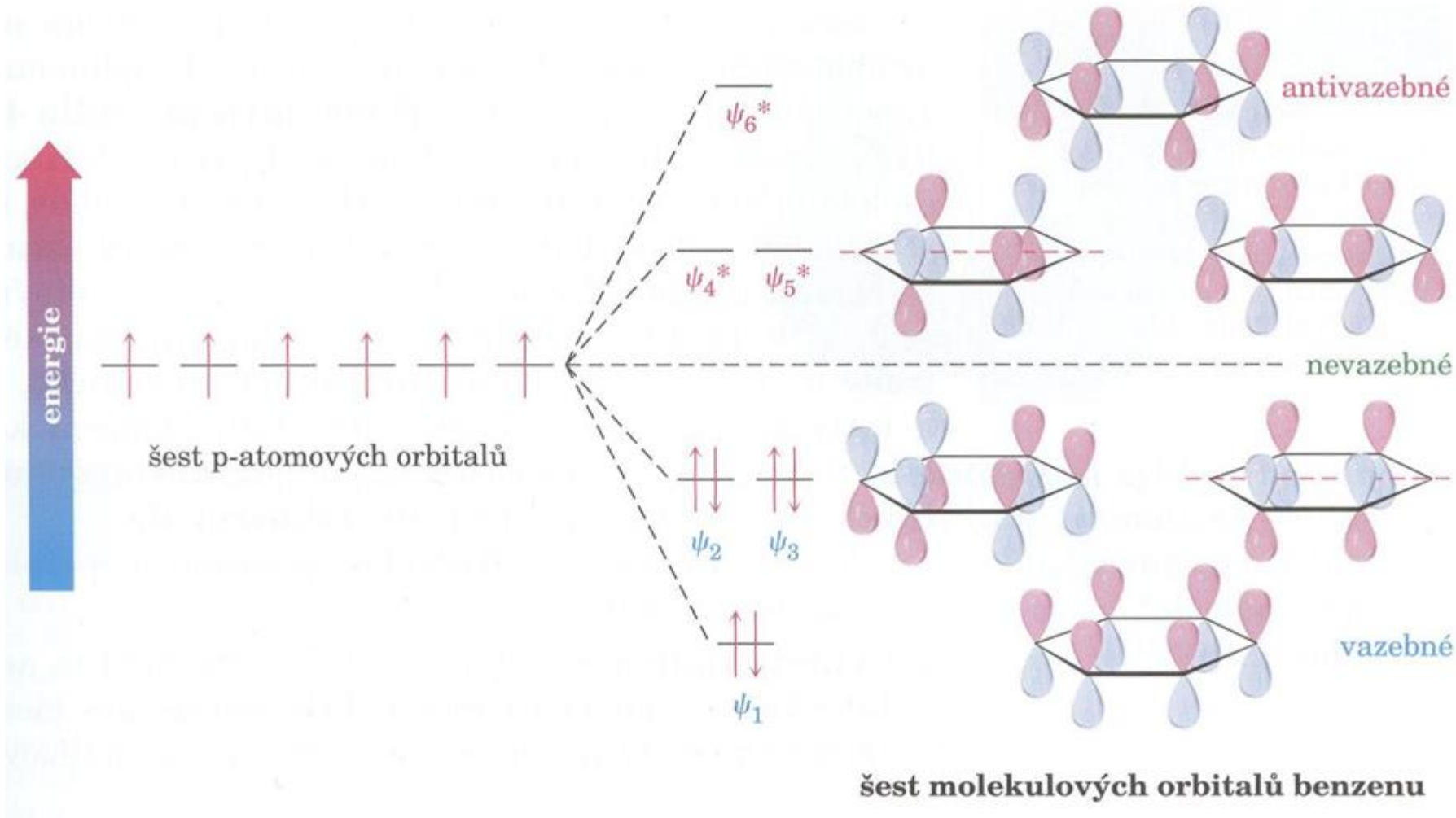



is the same as

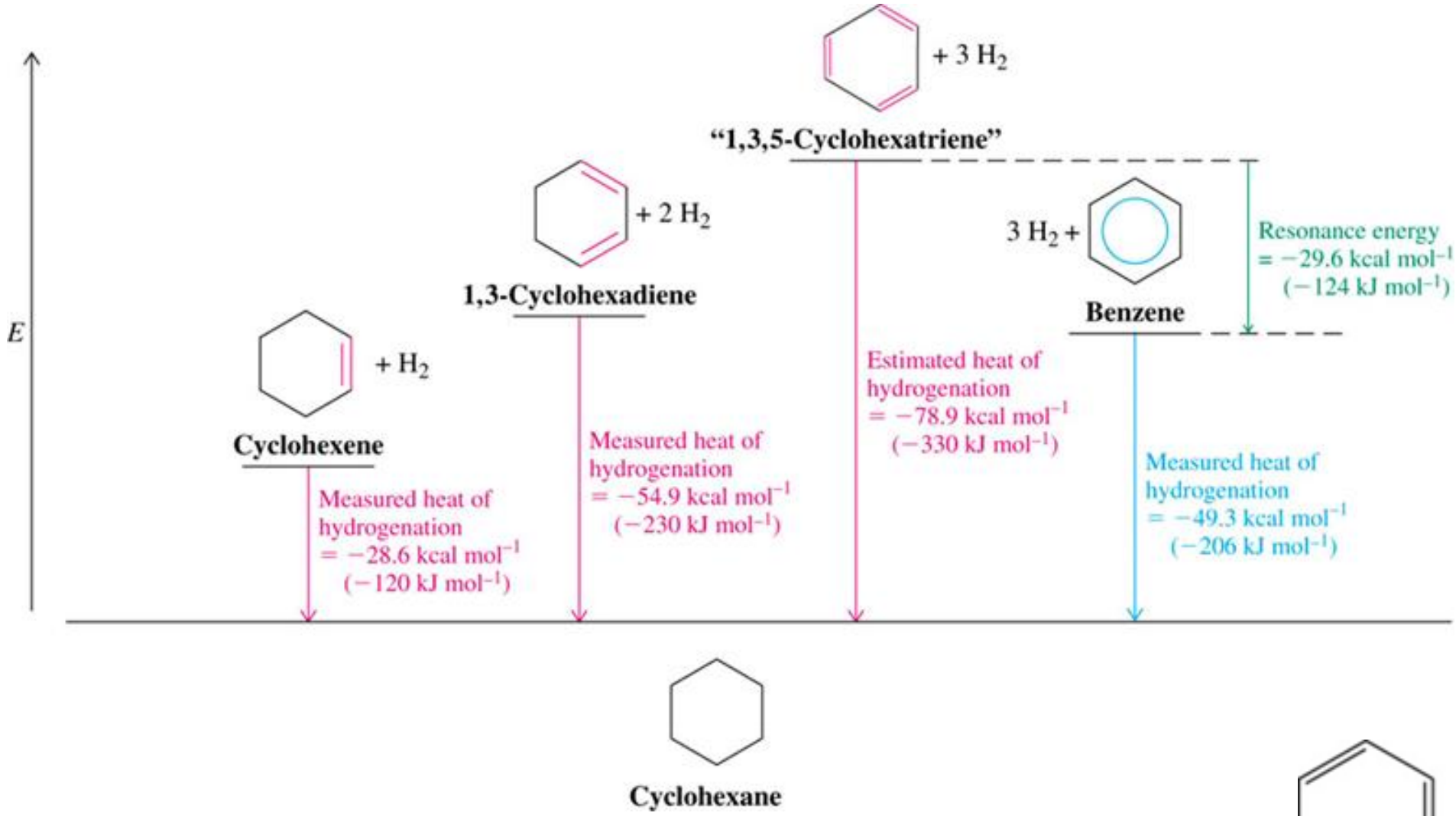


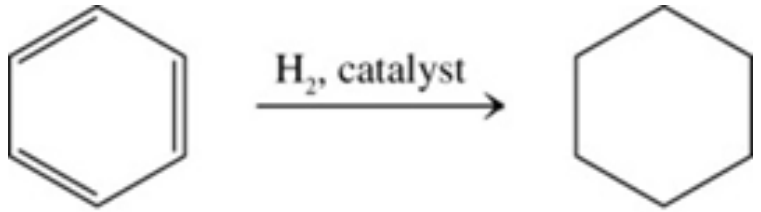






**šest molekulových orbitalů benzenu**




$\Delta H^\circ = -49.3$ kcal mol$^{-1}$

Resonance energy: ~−30 kcal mol$^{-1}$

# Hückelovo pravidlo a aromaticita

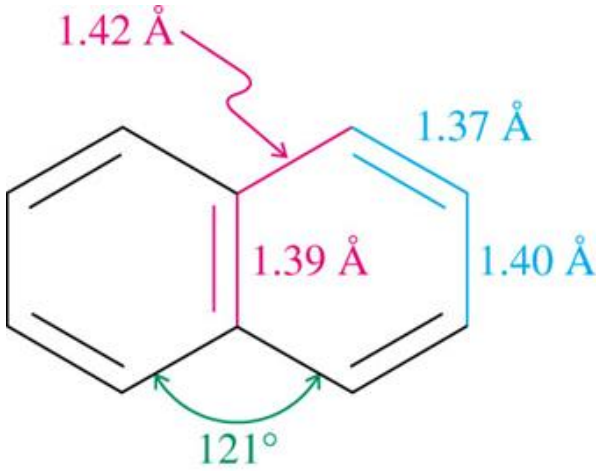
**Hückelovo pravidlo**

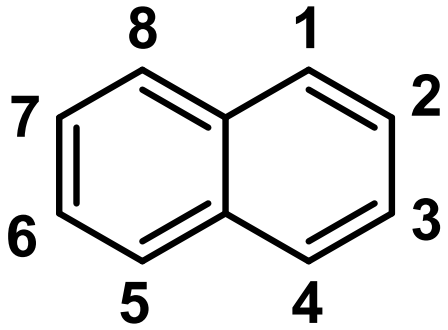
**Planární cyklické** systémy s **(4n+2) konjugovanými p elektrony** (n = 0, 1, 2 atd.),
tj. systémy s 2, 6, 10, 14, atd. konjugovanými **p** elektrony, jsou **aromatické.**
**Delokalizace p elektronů systém stabilizuje.**

**Planární cyklické** systémy s **4n konjugovanými p elektrony**, tj. systémy s 4, 8, 12, 16, atd. konjugovanými **p** elektrony, jsou **antiaromatické.**
**Delokalizace p elektronů by systém destabilizovala (nejsou delokalizovány).**

**Neplanární nebo acyklické** systémy s **nekonjugovanými p elektrony**, jsou **nearomatické.**
**Delokalizace p elektronů v těchto systémech není možná,.**

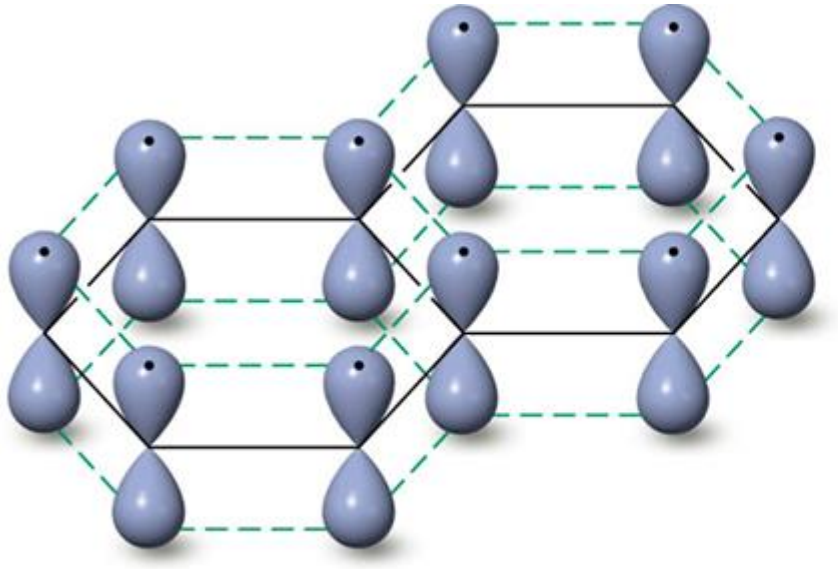
# Naftalen



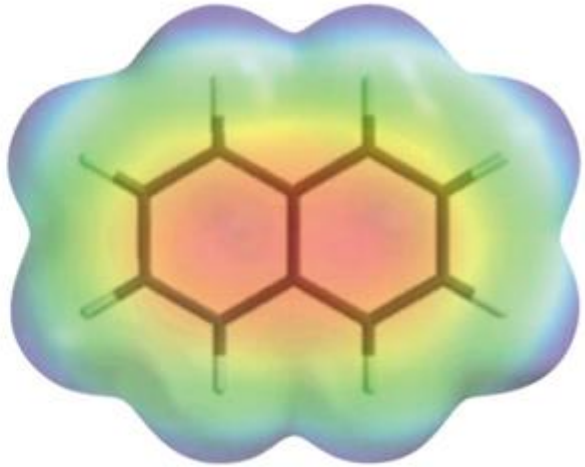




**10 (4 x 2 + 2) π elektronů**

**Aromatický**



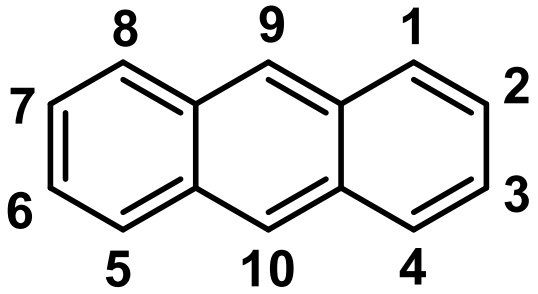
A



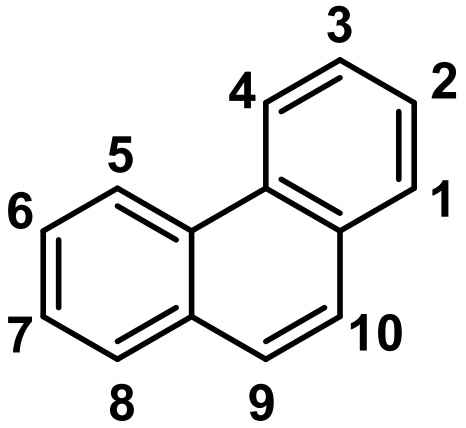
B

# Kondenzované aromatické sloučeniny

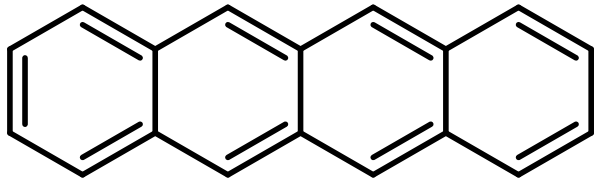
**Anthracen**



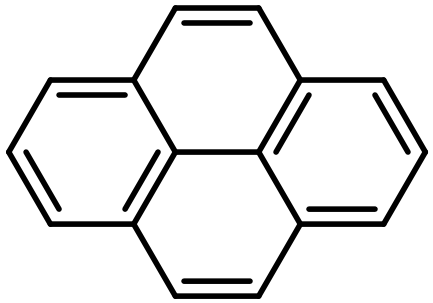

**Fenanthren**



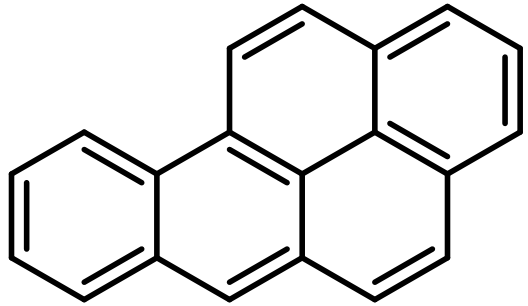

**Tetracen**



**Pyren**

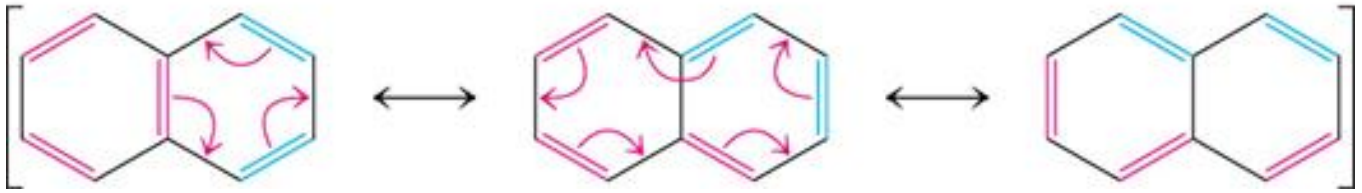


**Benzo[a]pyren**

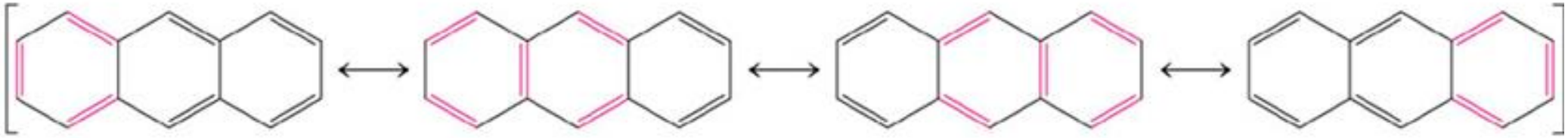


# Rezonance v kondenzovaných aromatických sloučeninách

**Resonance Forms of Naphthalene**

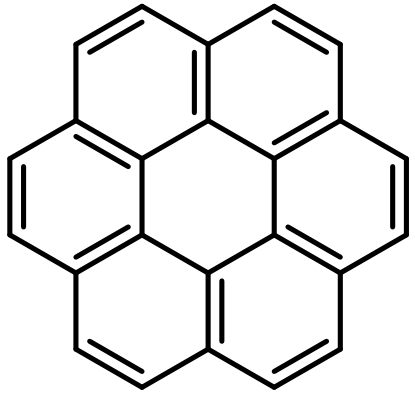


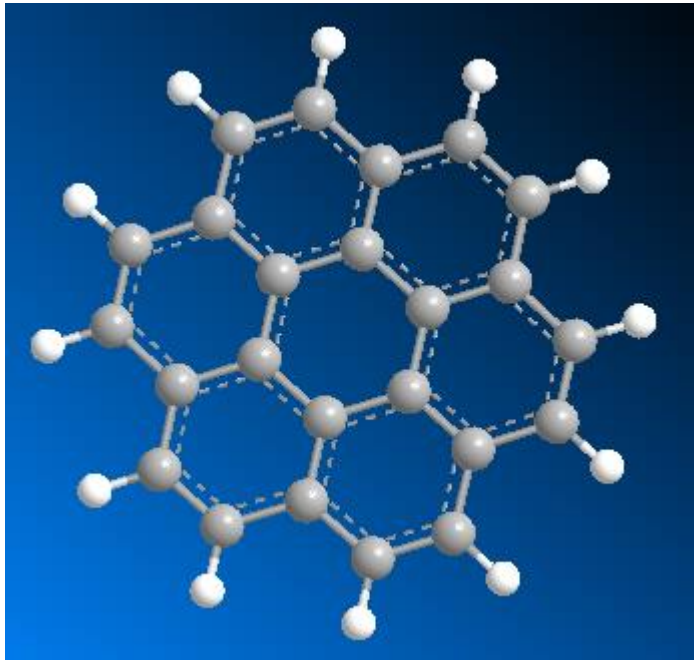
**Resonance in Anthracene**



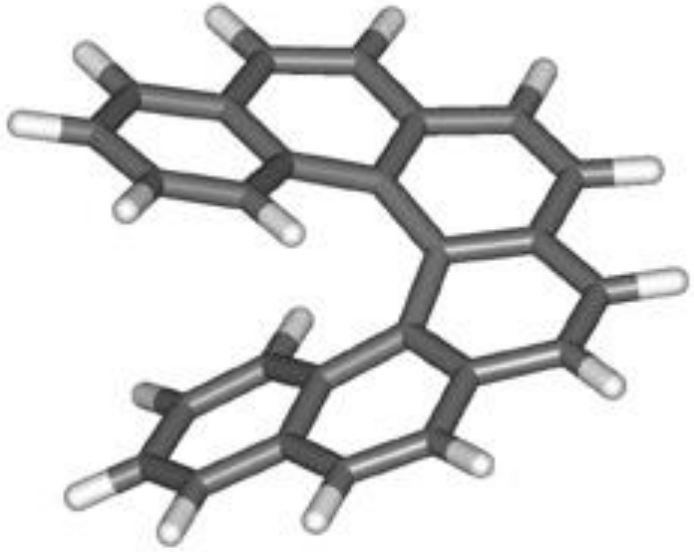
**Resonance in Phenanthrene**

## Koronen

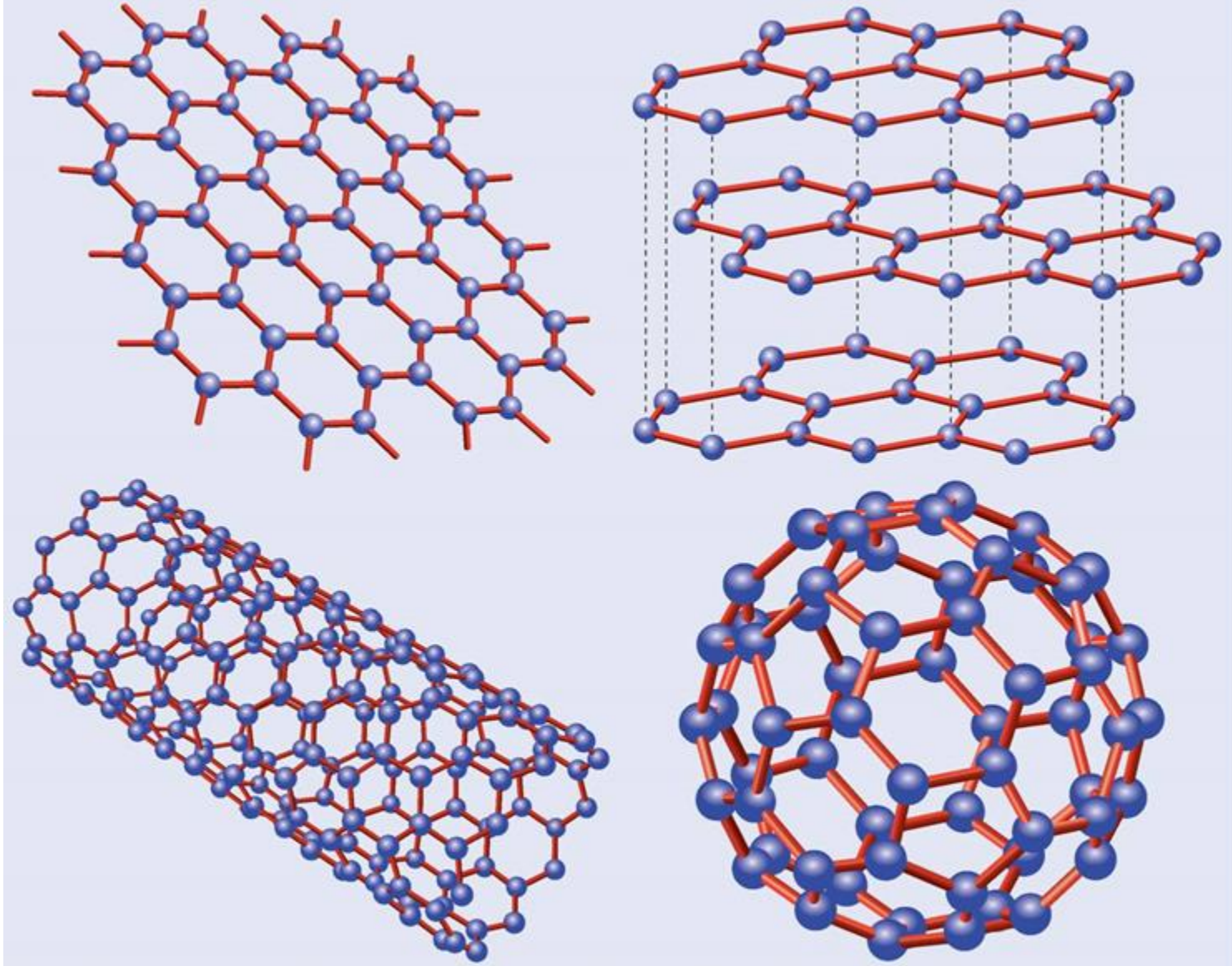




## [6]-Helicen



## 2 Graphene: mother of them all

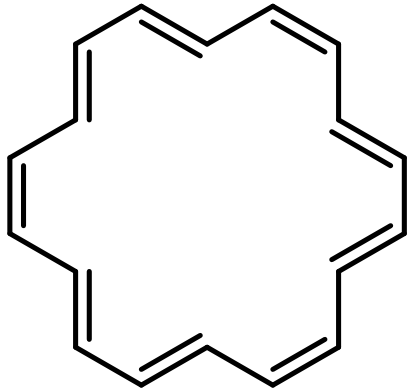


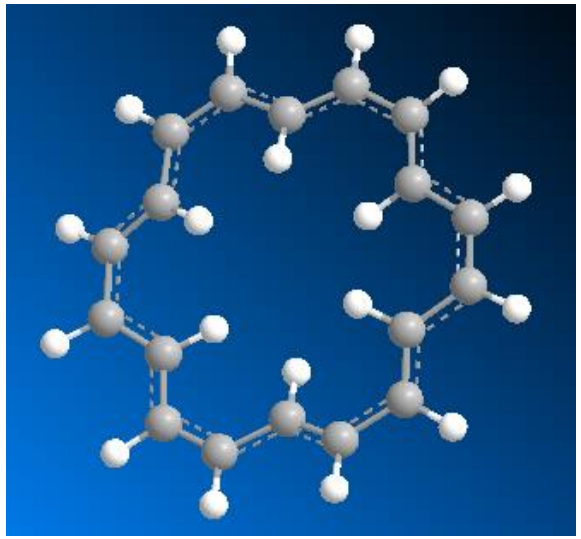
Graphene (top left) consists of a 2D hexagonal lattice of carbon atoms. Each atom is covalently bonded to three others; but since carbon has four valence electrons, one is left free – allowing graphene to conduct electricity. Other well-known forms of carbon all derive from graphene: graphite is a stack of graphene layers (top right); carbon nanotubes are rolled-up cylinders of graphene (bottom left); and a buckminsterfullerene ($C_{60}$) molecule consists of graphene balled into a sphere by introducing some pentagons as well as hexagons into the lattice (bottom right).

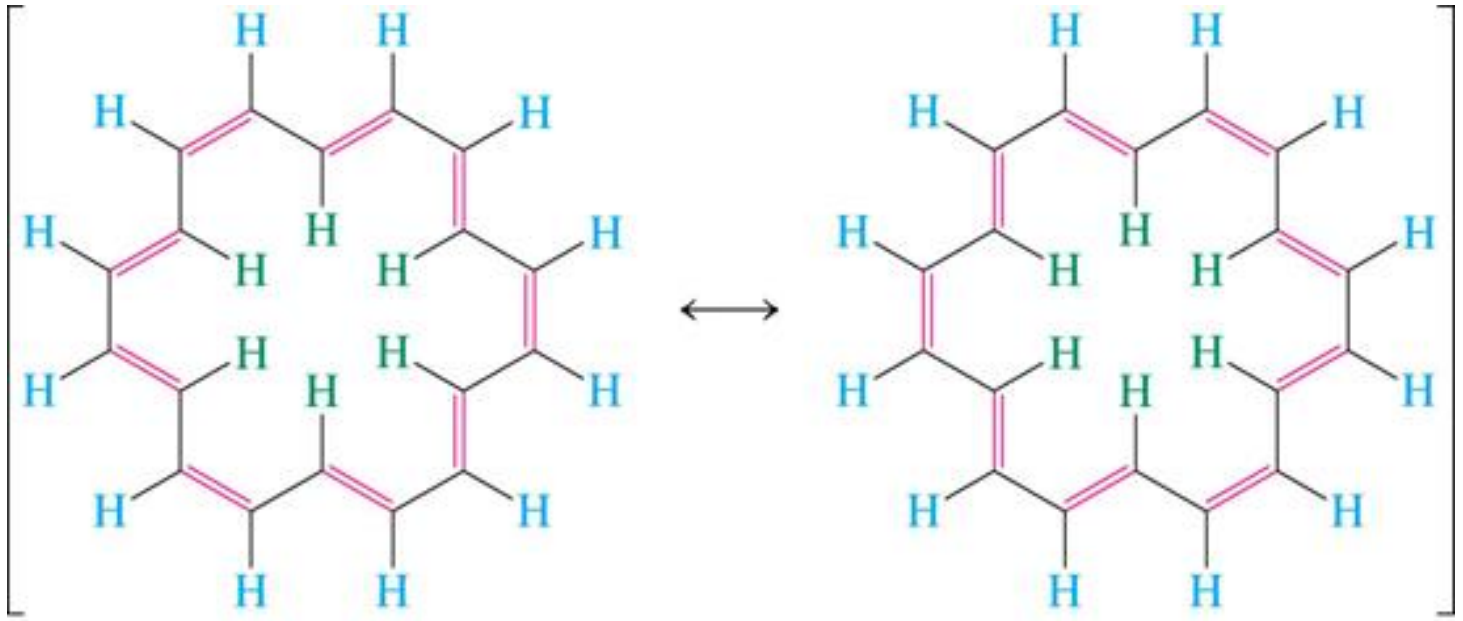
# [18]anulen (cyklooktadeka-1,3,5,7,9,11,13,15,17-nonaen)

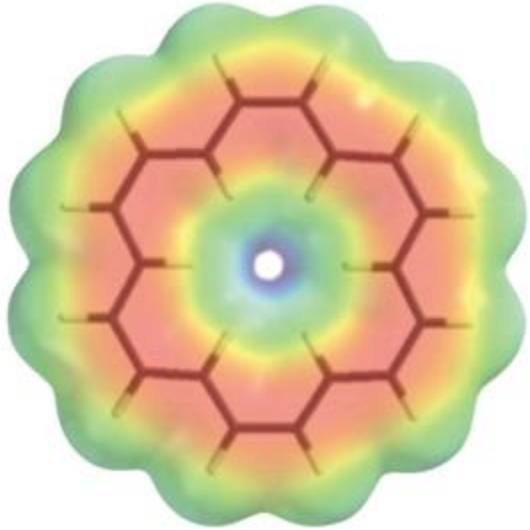
**18 (4 x 4 + 2) π elektronů**

**Aromatický**





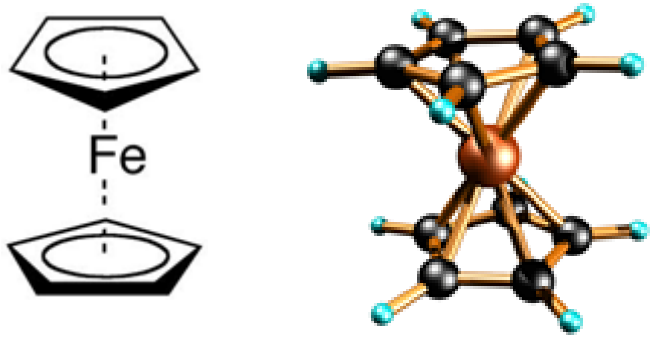


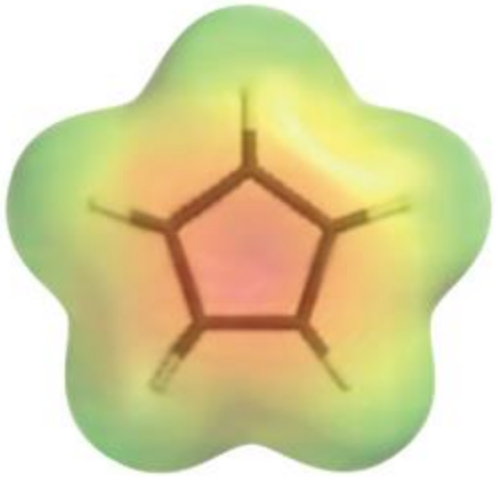


# Cyklopentadienylový anion

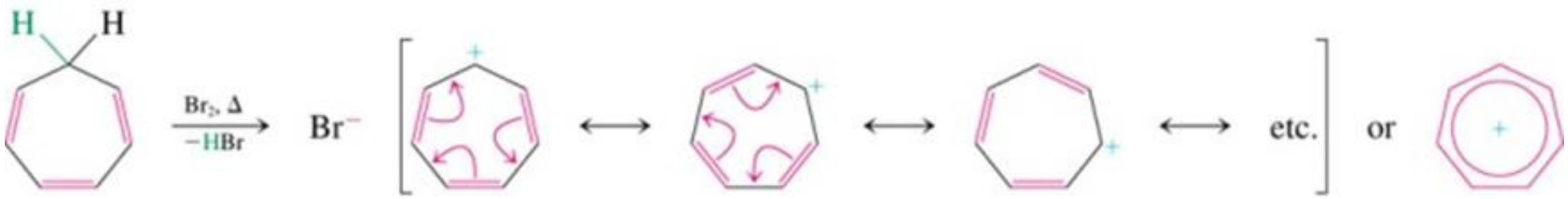

**6 π elektronů**
**Aromatický**

**Ferrocen**

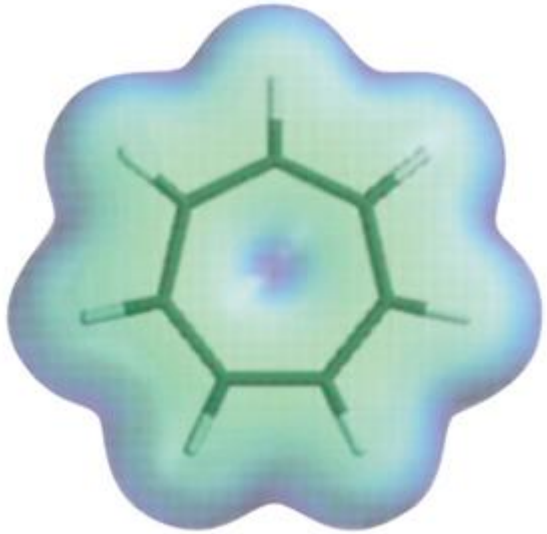


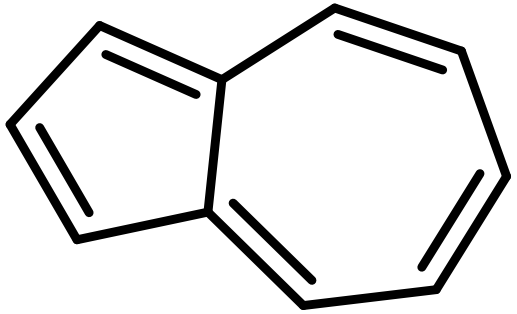
# Cykloheptatrienový kation (tropylium)

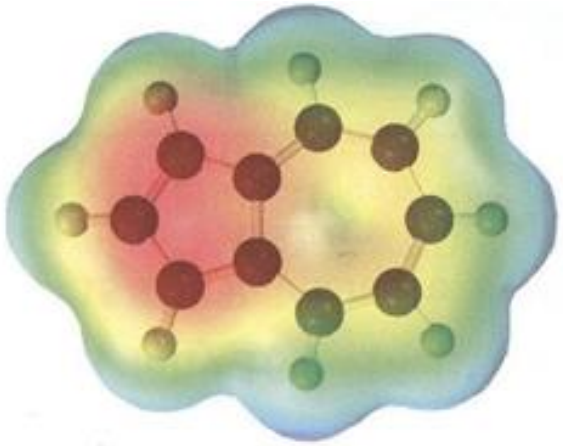


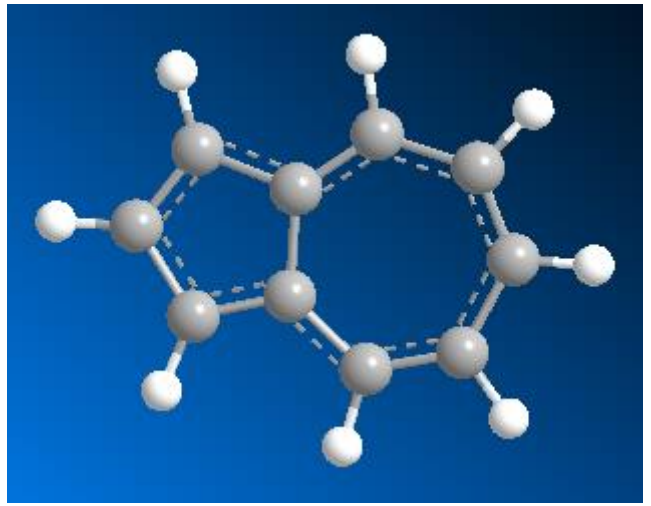

**6 π elektronů**
**Aromatický**



# Azulen







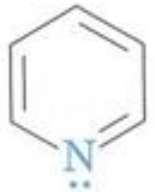
**10 π elektronů**

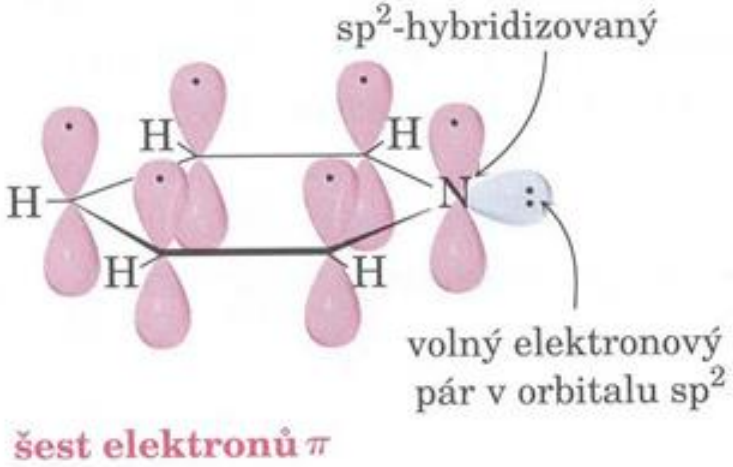
**Aromatický**

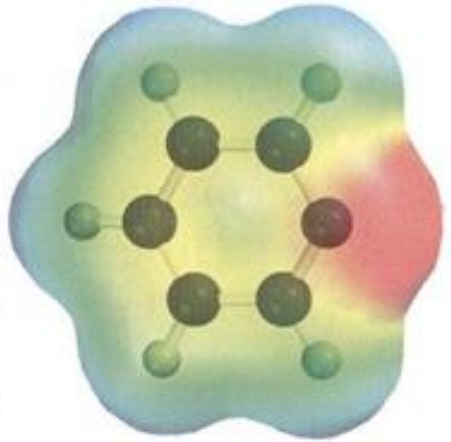

*Lactarius indigo* obsahuje (7-isopropenyl-4-methylazulen-1-yl)methyl stearate.

# Heteroaromatické sloučeniny

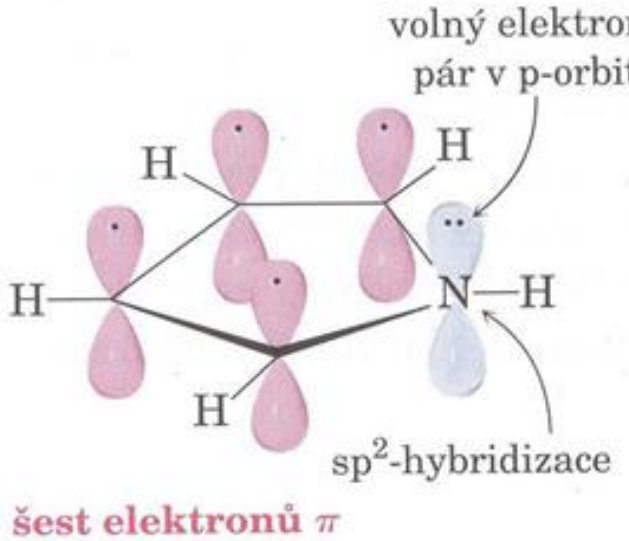
**Pyridin**

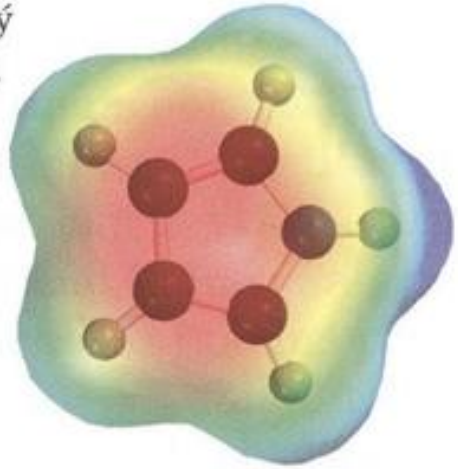


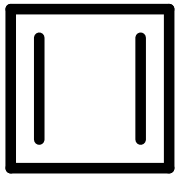



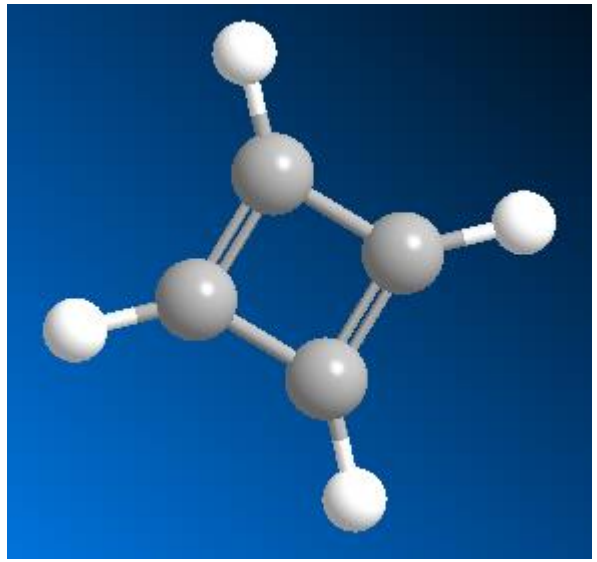
**Pyrrol**

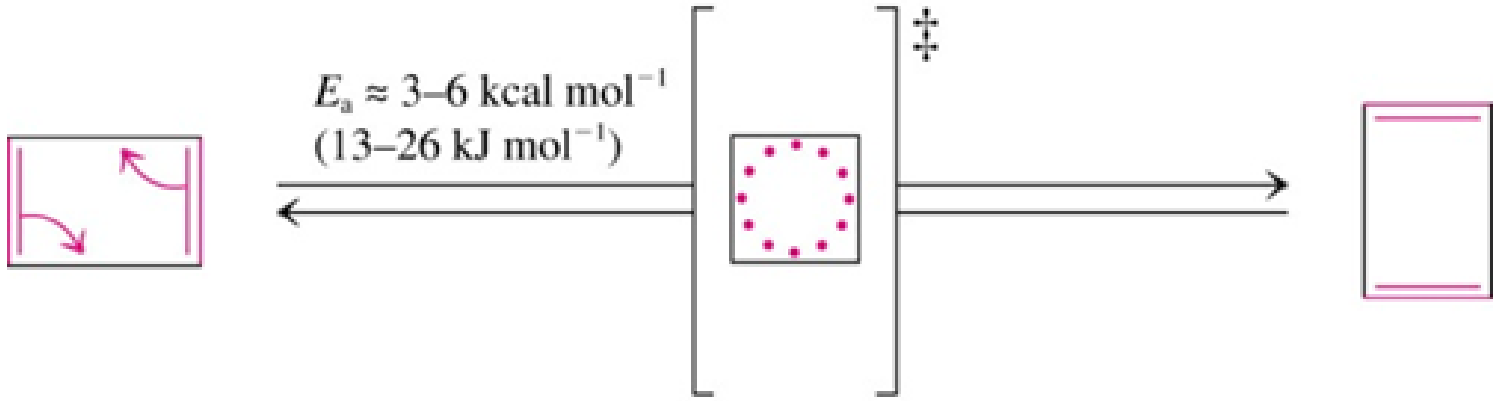
# Cyklobutadien



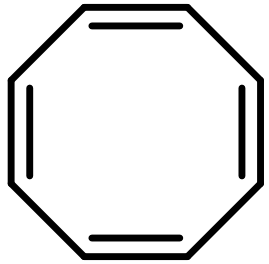


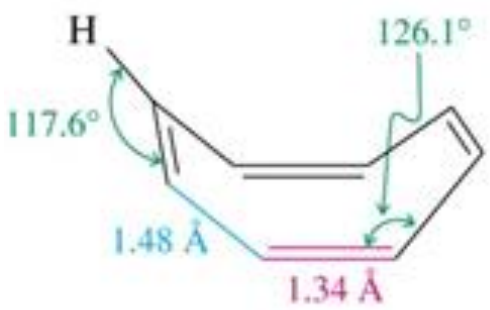
**4 π elektronů**

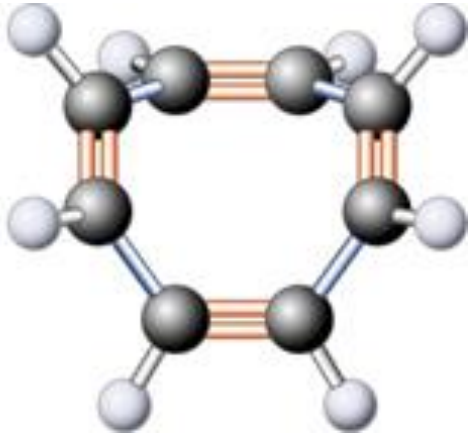
**Antiaromatický**

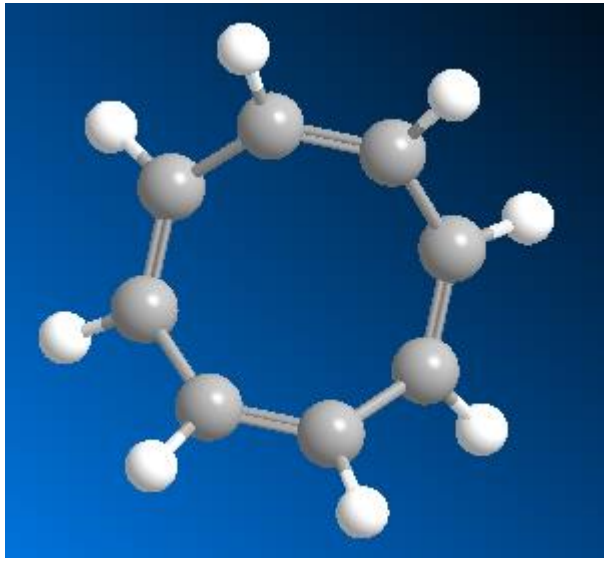


# Cyklookta-1,3,5,7-tetraen



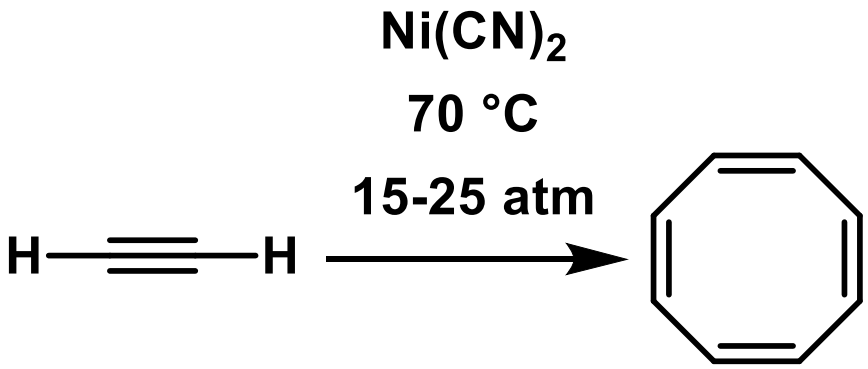


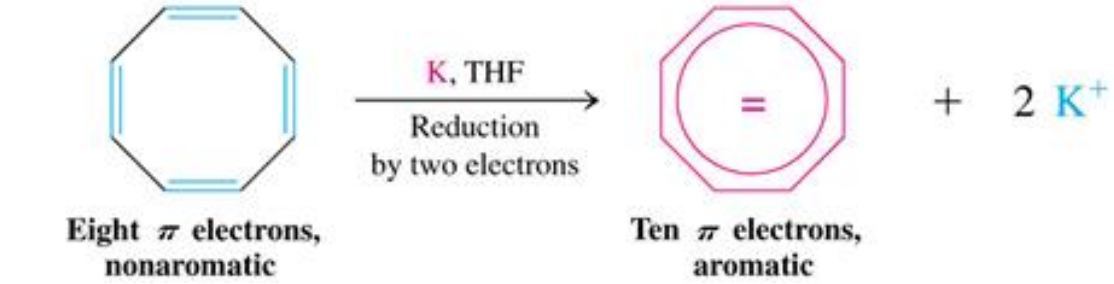


**4 π elektronů**

**Nearomatický**




**Nonaromatic Cyclooctatetraene Forms an Aromatic Dianion**



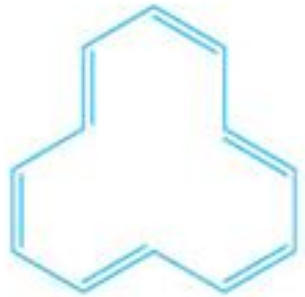
# The Annulenes and Other Cyclic Polyenes

Cyclobutadiene:
planar, antiaromatic

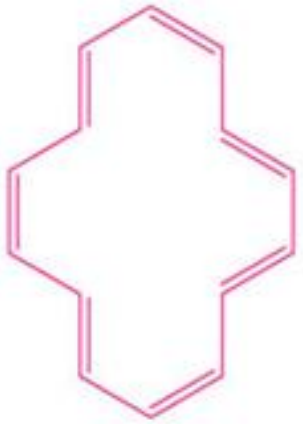
Benzene:
planar, aromatic

Cyclooctatetraene:
nonplanar = nonaromatic

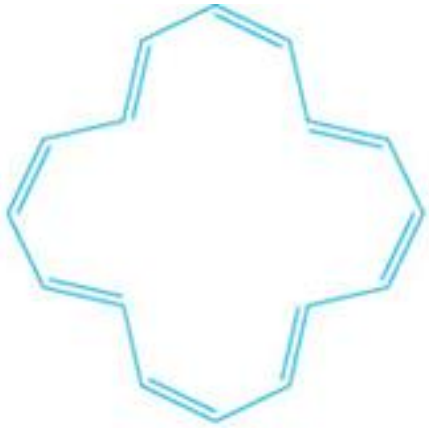
[10]Annulene:
nonplanar = nonaromatic



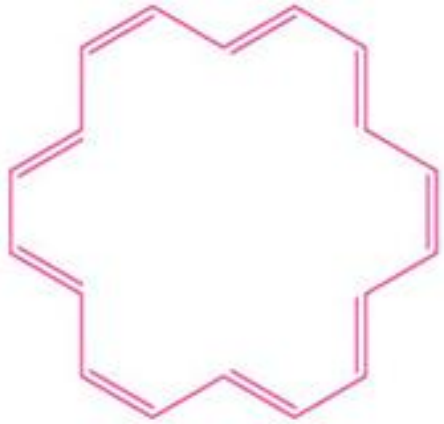
[12]Annulene:
planar = antiaromatic



[14]Annulene:
planar = aromatic



[16]Annulene:
planar = antiaromatic



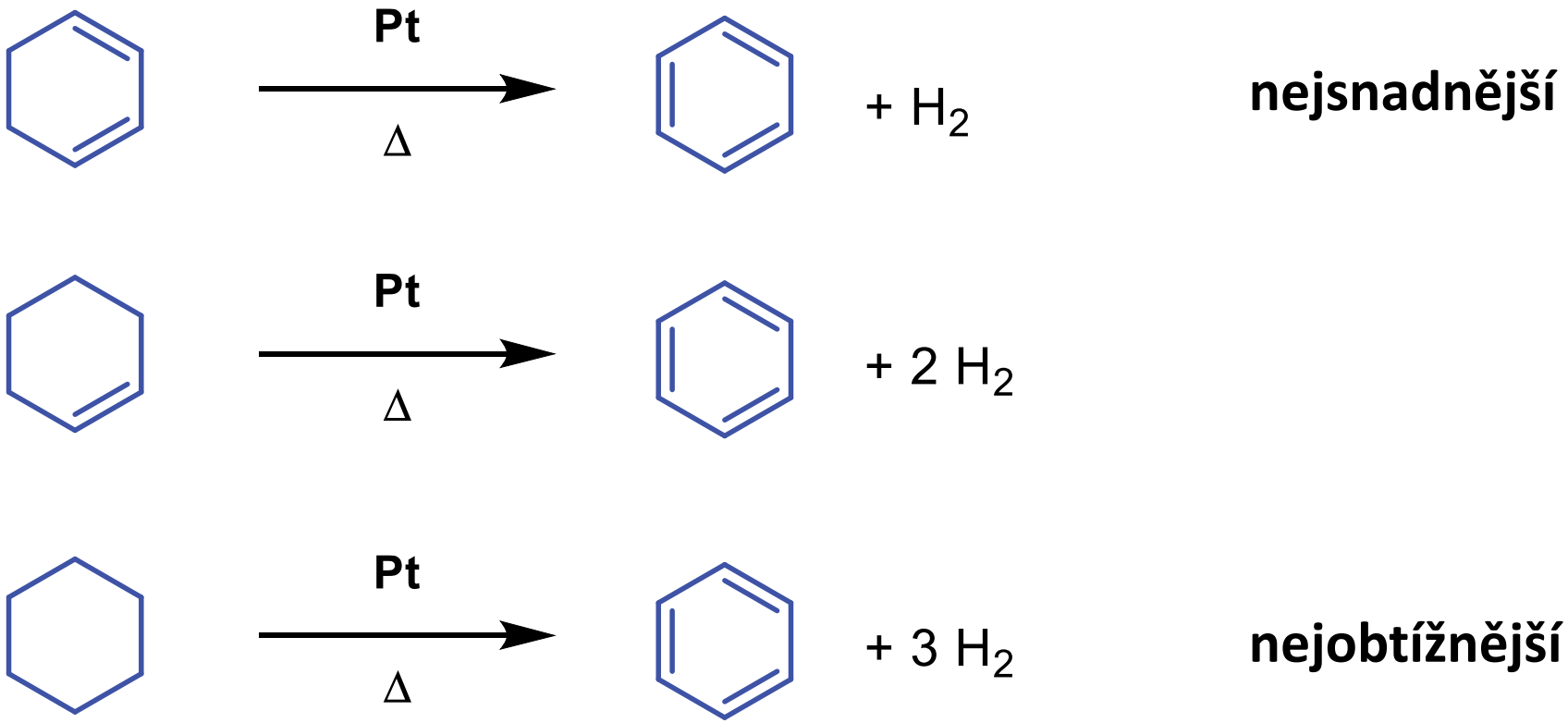
[18]Annulene:
planar = aromatic

1,3-Cyclopentadiene:
noncyclically delocalized
= nonaromatic

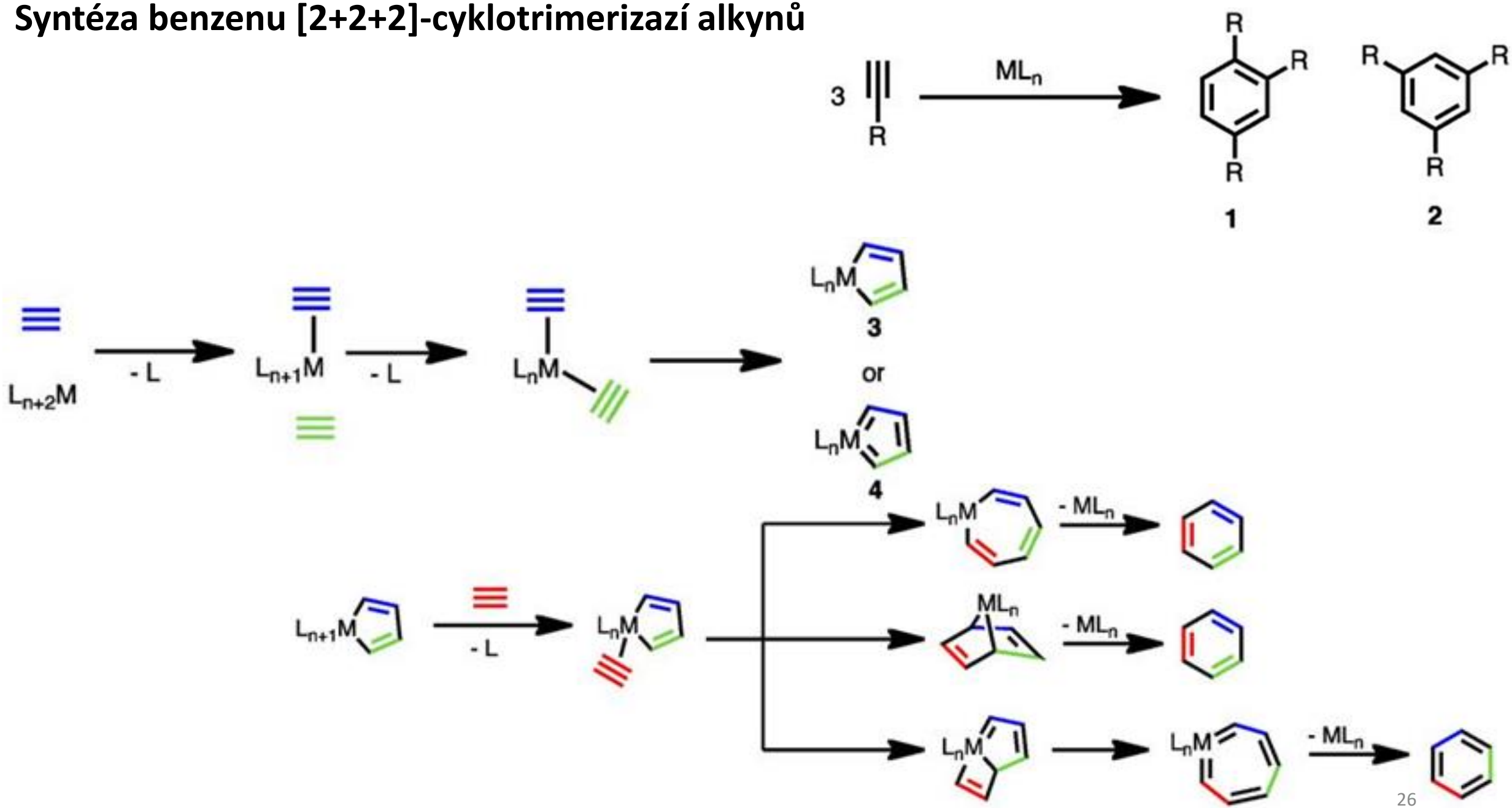
1,4-Cyclohexadiene:
nondelocalized
= nonaromatic

# Syntéza benzenu a dalších aromátů

## Kalalytická dehydrogenace

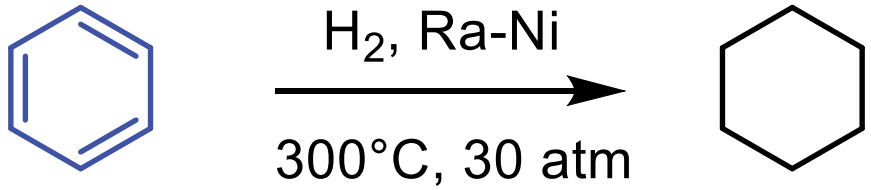


# Syntéza benzenu [2+2+2]-cyklotrimerizací alkynů

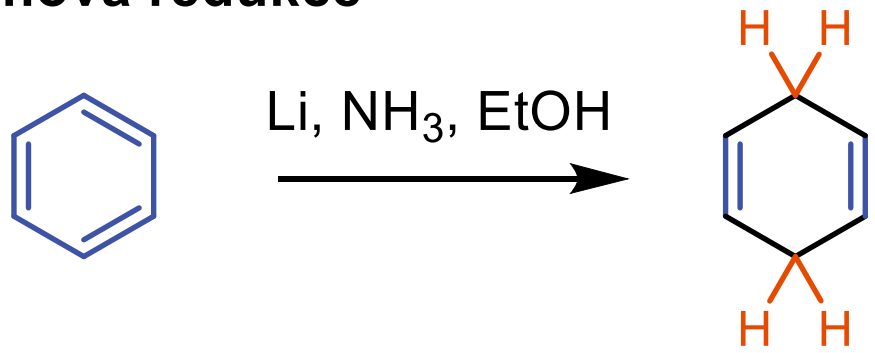


# Reaktivita benzenu – redukce (velmi obtížně)

## Kalalytická hydrogenace

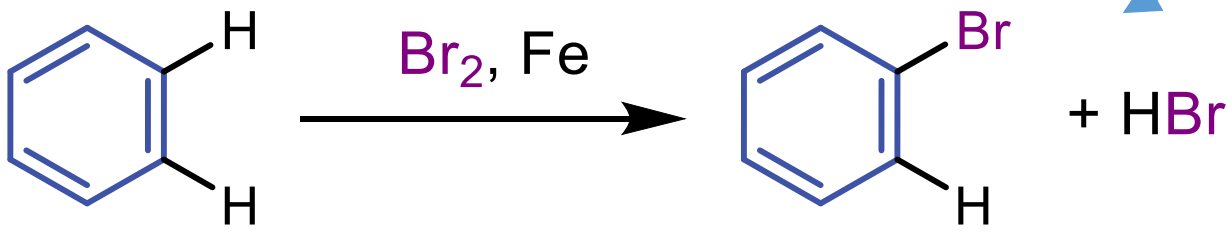



## Birchova redukce

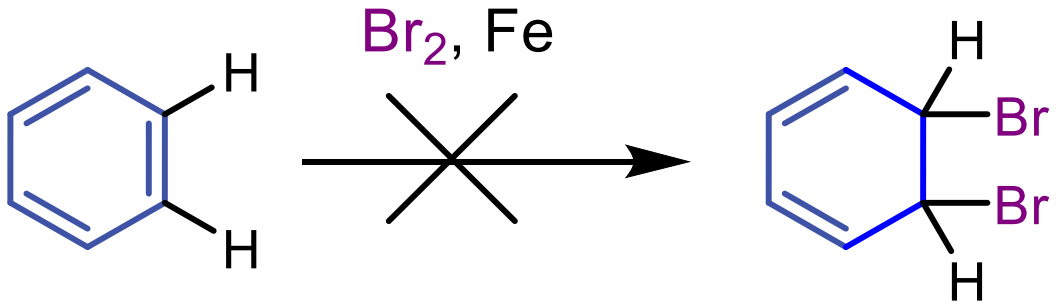


# Reaktivita benzenu – elektrofilní substituce vs. adice

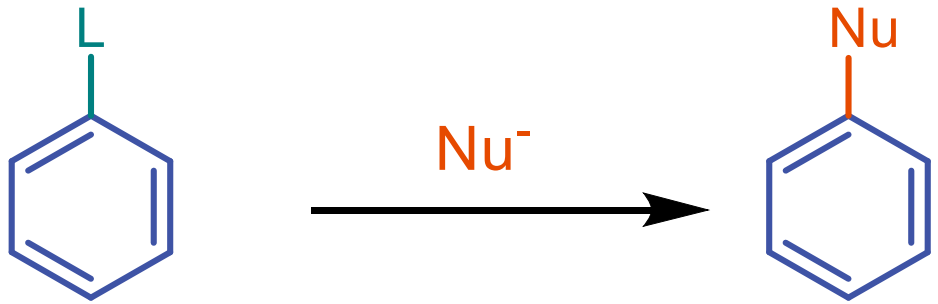
## Elektrofilní substituce probíhají snadno



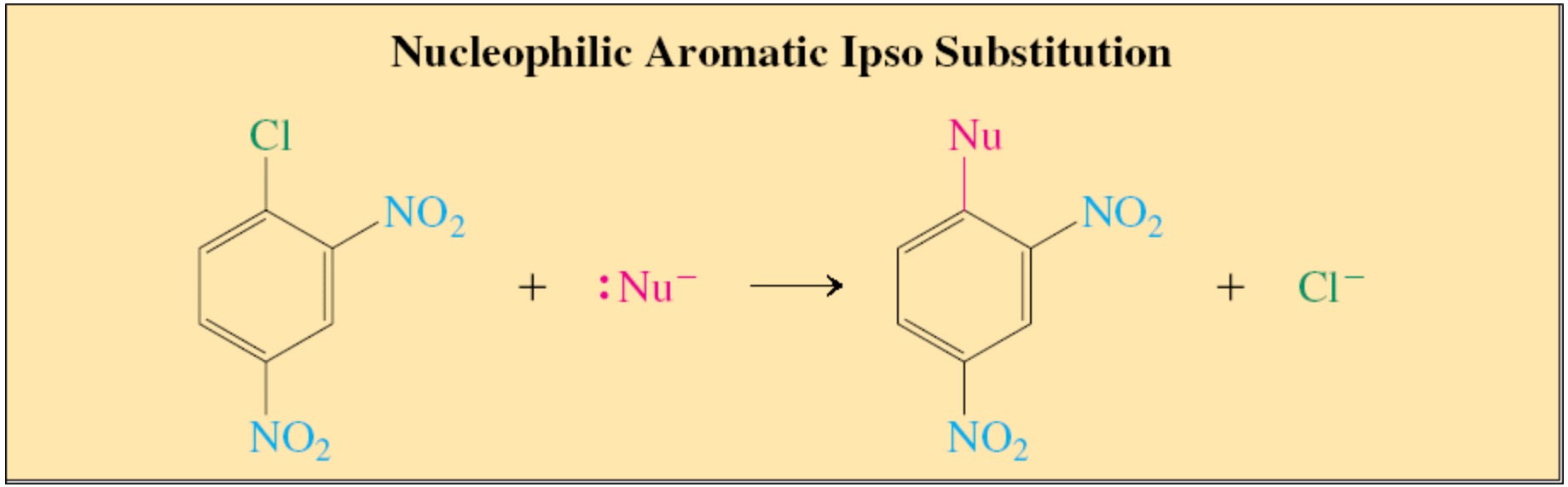

## Adiční reakce neprobíhají

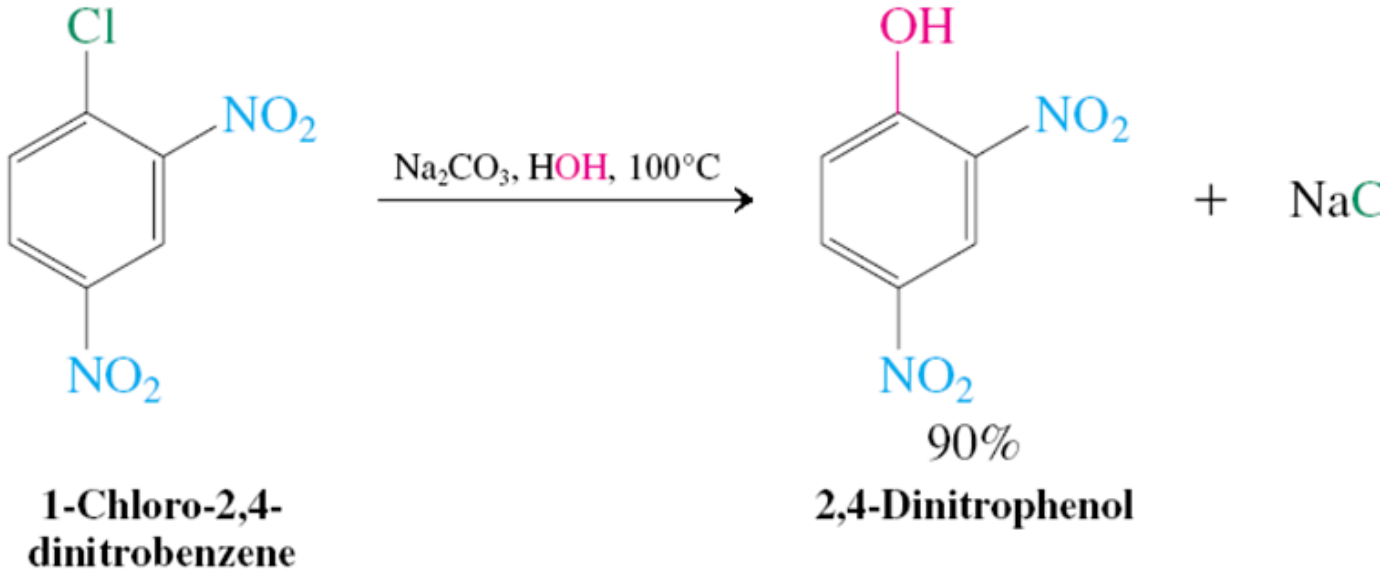


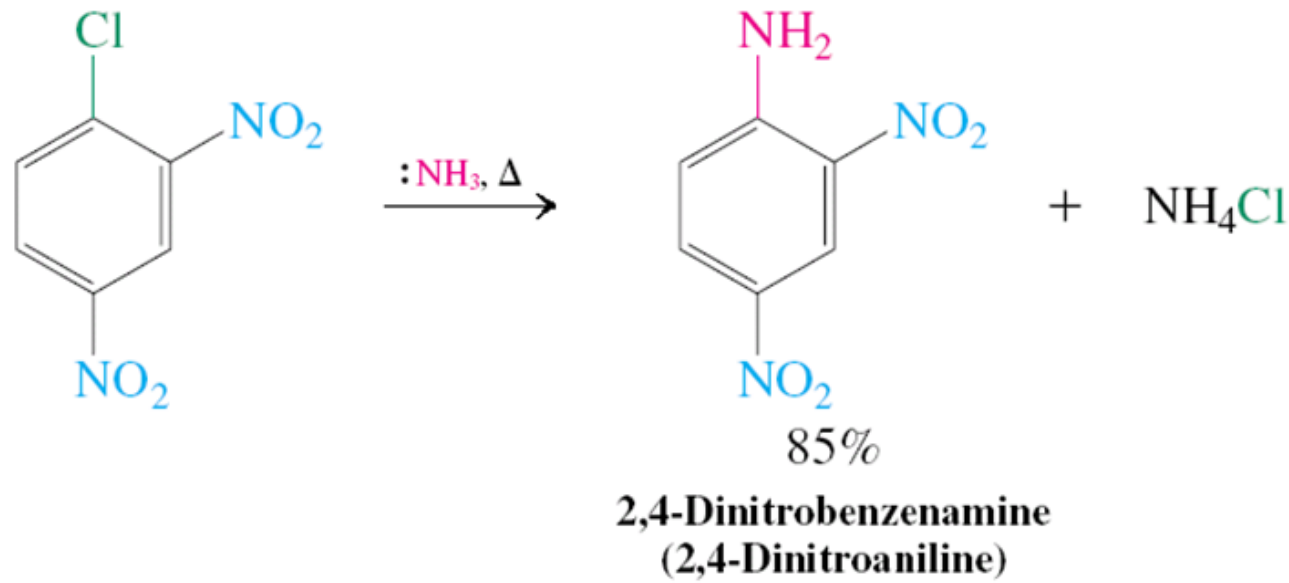

## Nukleofilní substituce probíhají obtížně – pouze pro elektronově chudší systémy



# Nukleofilní substituce probíhají obtížně – pouze pro elektronově chudší systémy

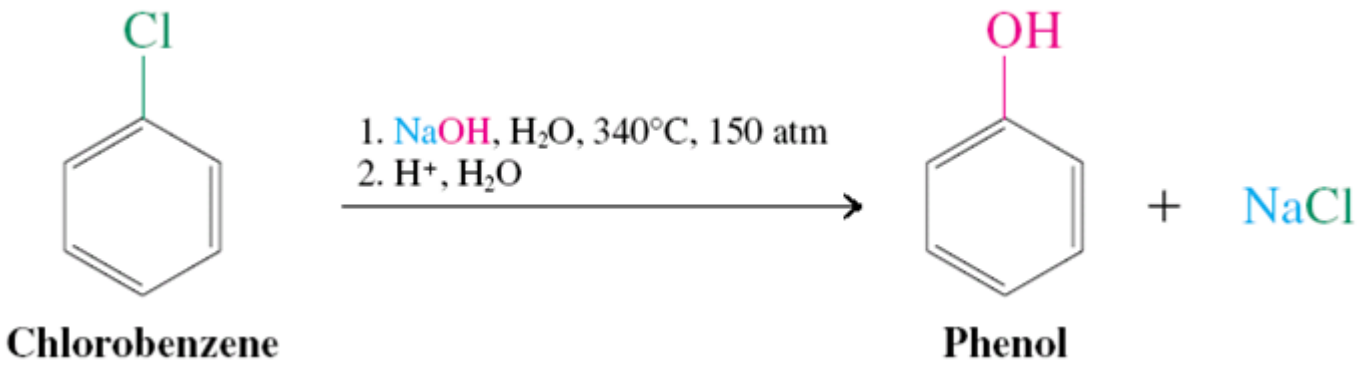


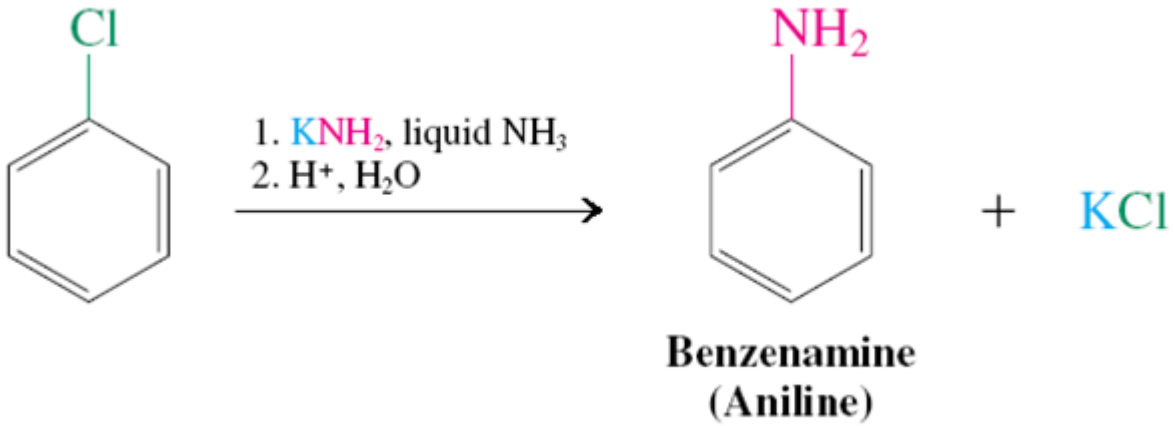

Cl
NO2
NO2
Na2CO3, HOH, 100°C
OH
NO2
NO2
+ NaC
90%
1-Chloro-2,4-dinitrobenzene
2,4-Dinitrophenol

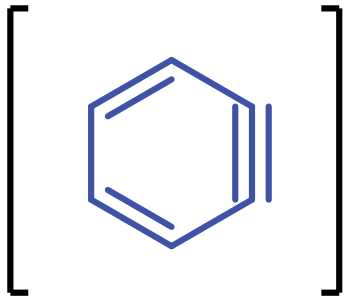

Cl
NO2
NO2
:NH3, Δ
NH2
NO2
NO2
+ NH4Cl
85%
2,4-Dinitrobenzenamine
(2,4-Dinitroaniline)

# Nukleofilní substituce elektronově-bohatých halogenarenů

Halogenareny bez elektron-odtahujících skupin mohou poskytovat nukleofilní substituci za vysokých teplot a tlaků – tato reakce probíhá před benzynový intermediát.



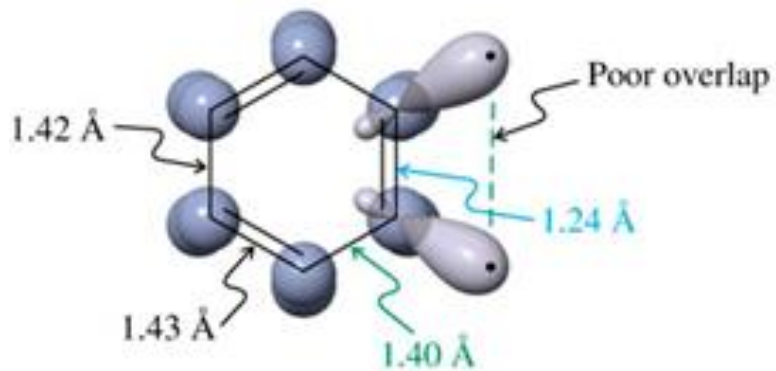
## Mechanism of Nucleophilic Substitution of Simple Haloarenes

**Step 1.** Elimination occurs stepwise

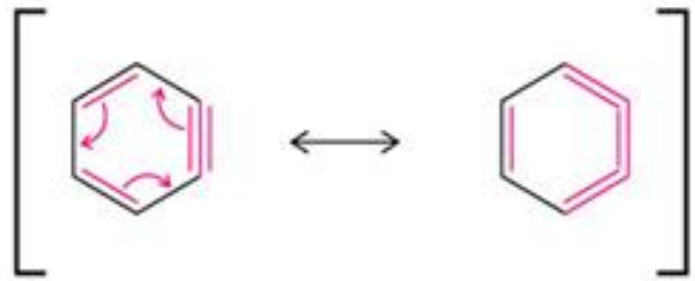

**Phenyl anion**
(Intermediate)

**Benzyne**
(Reactive intermediate; not isolated)

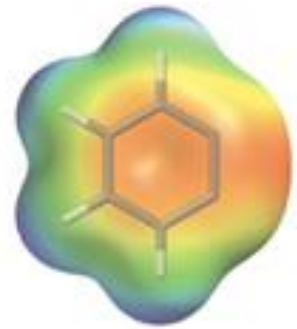
**Step 2.** Addition occurs to both strained carbons




A



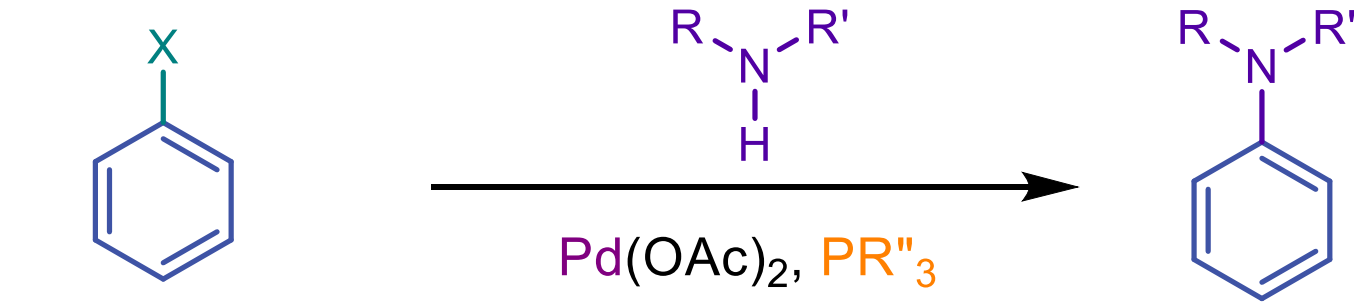
B



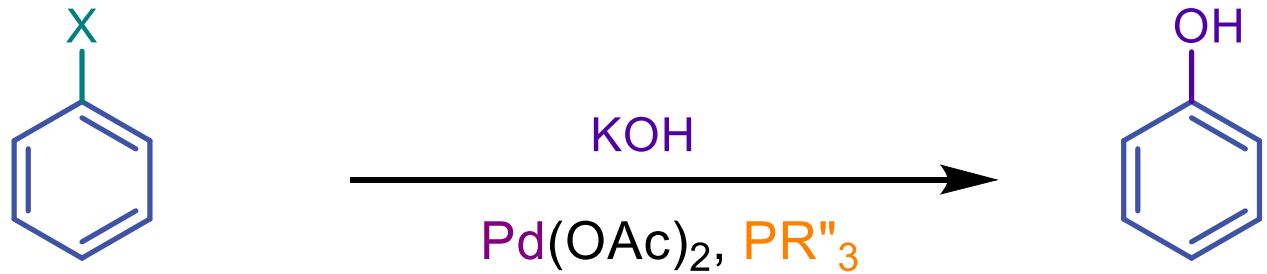
C

# Moderní katalytické metody „nukleofilní substituce“ halogenarenů

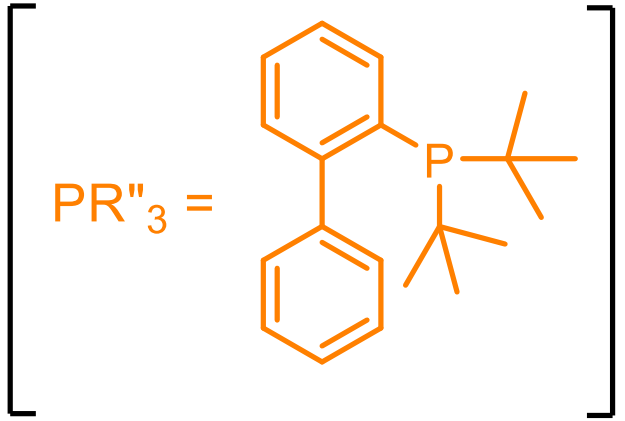
- Pd-katalyzované C-X cross-couplingy (Buchwald-Hartwigovy reakce)




X = I > Br > Cl



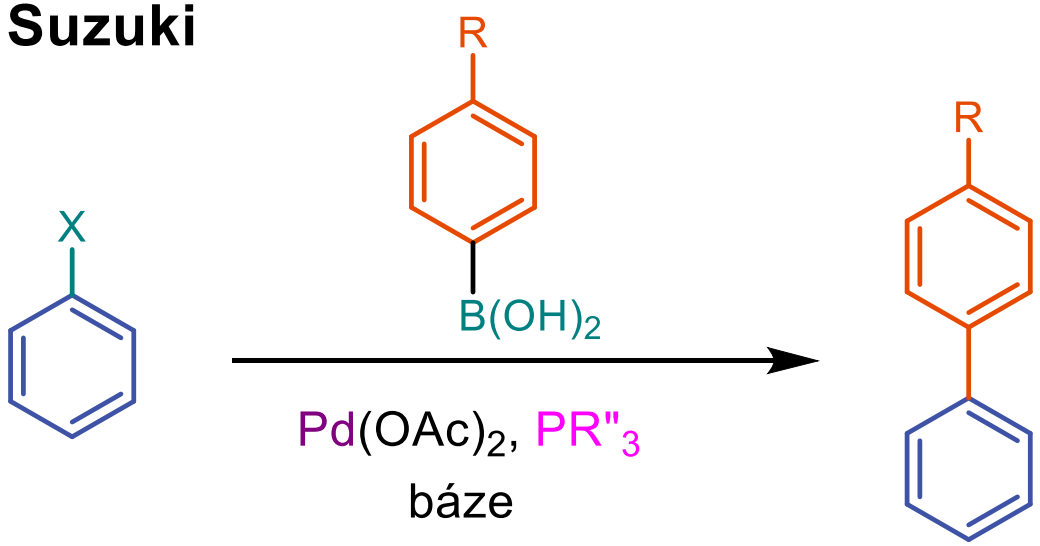

X = I > Br > Cl



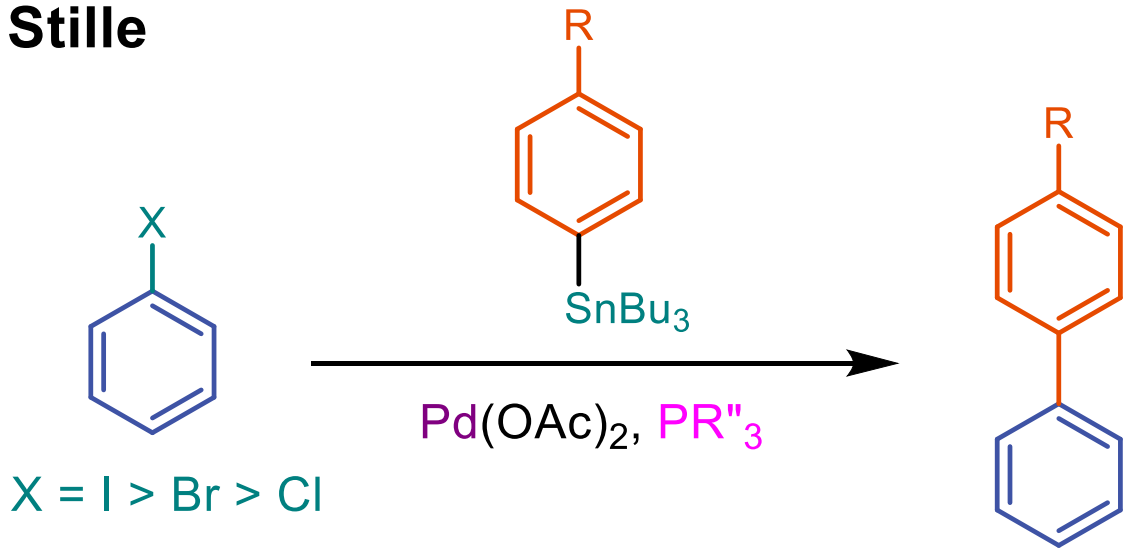
# Moderní katalytické metody „nukleofilní substituce“ halogenarenů

- Pd-katalyzované C-C cross-couplingy (Suzukiho, Negishiho nebo Stilleho reakce)

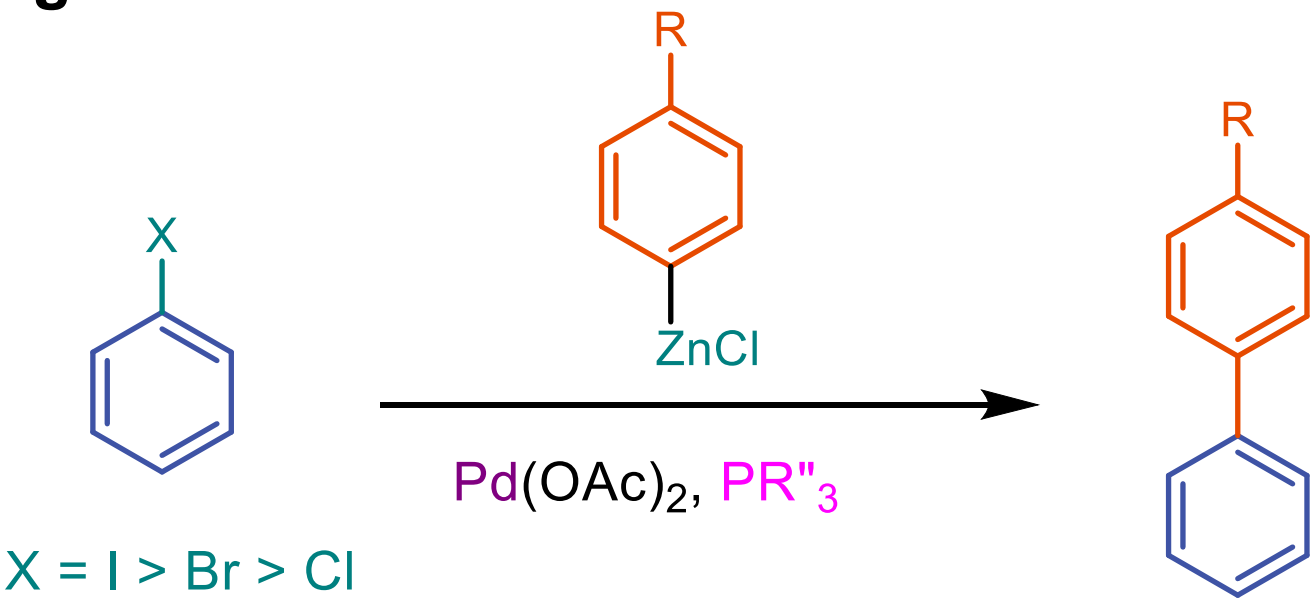
**Suzuki**




**Stille**



## Negishi




X = I > Br > Cl

## Nobelova cena za chemii 2010