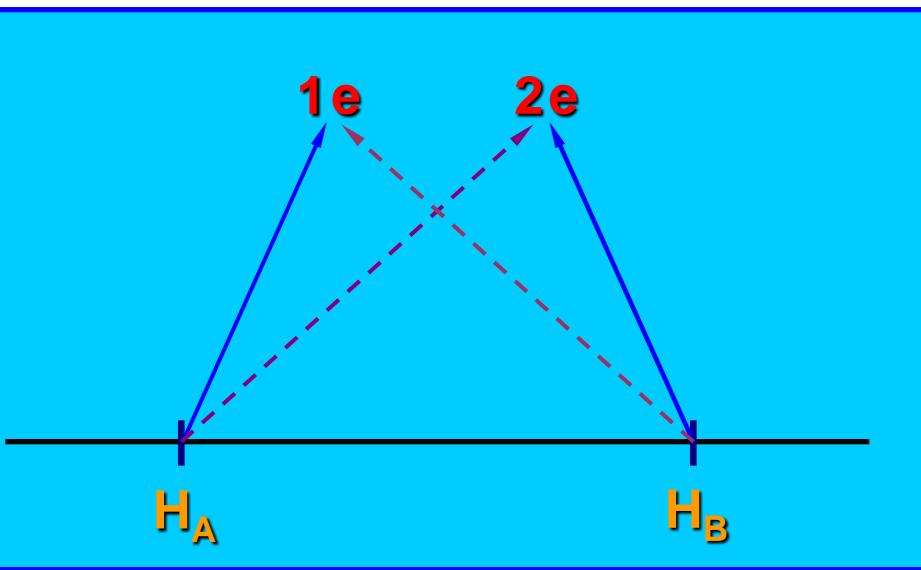


Chemická vazba teorie molekulových orbitalů (MO)

Lineární kombinace atomových orbitalů (LCAO)

$$\Psi = \phi_A(1)\phi_B(2) + \phi_A(2)\phi_B(1)$$



Coulombický integrál
Překryvový integrál
Resonanční integrál

Chemická vazba teorie molekulových orbitalů (MO)

Lineární kombinace atomových orbitalů (LCAO)

$$\Psi = \phi_A(1)\phi_B(2) + \phi_A(2)\phi_B(1)$$

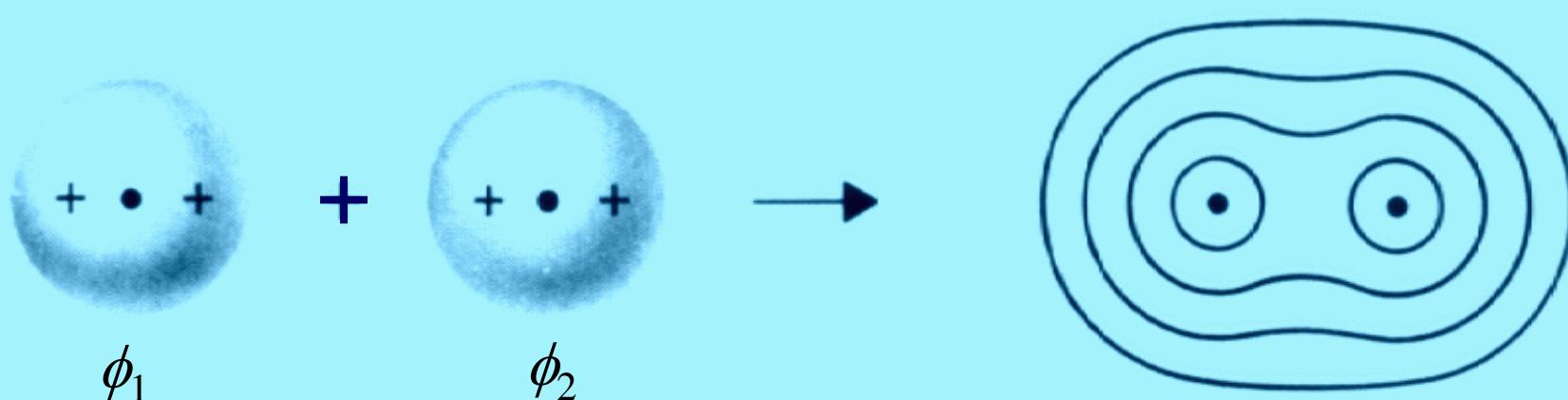
Výsledek kombinace – 2 řešení

vazebný MO

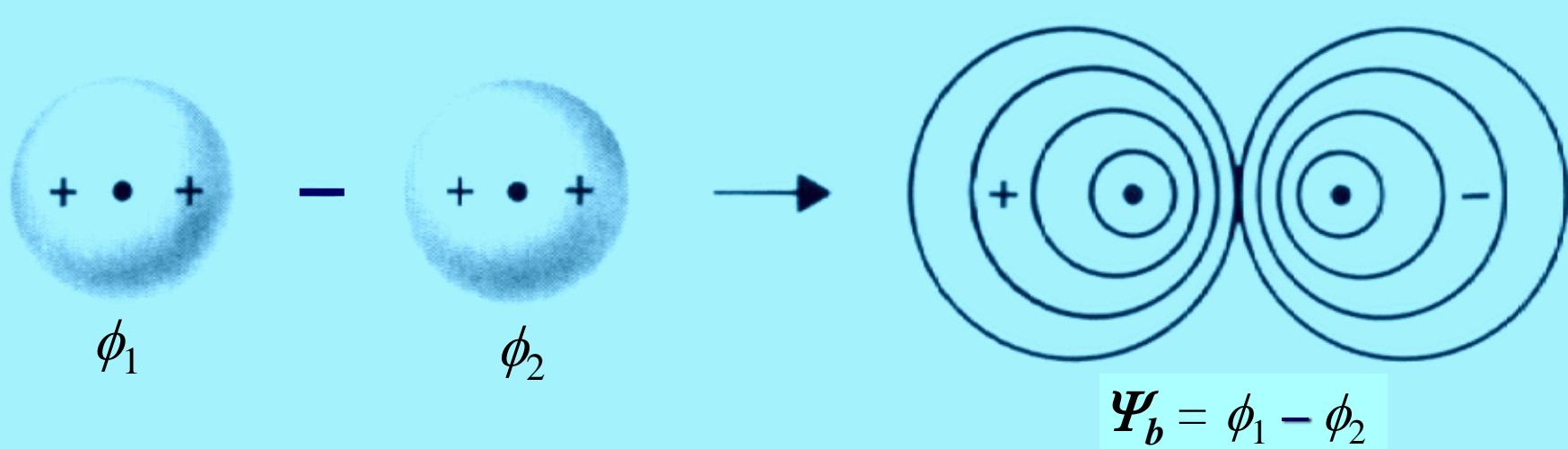
proti(anti)vazebný MO



MO-LCAO

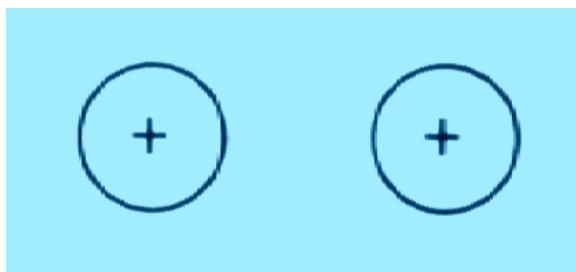


$$\Psi_a = \phi_1 + \phi_2$$

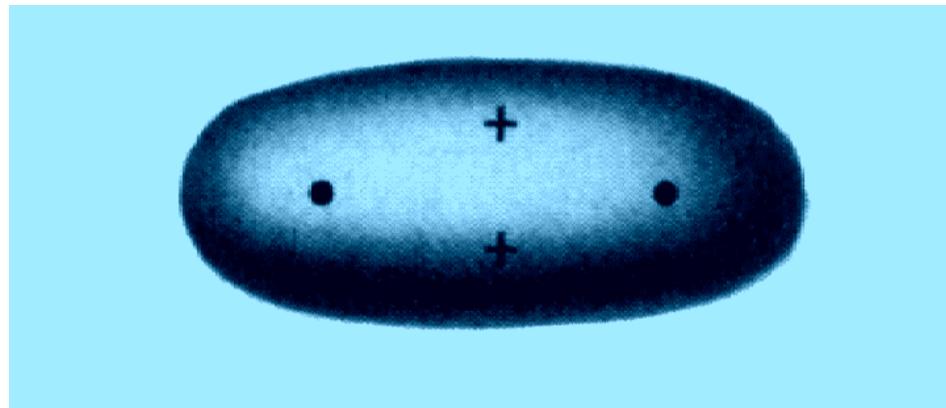


$$\Psi_b = \phi_1 - \phi_2$$

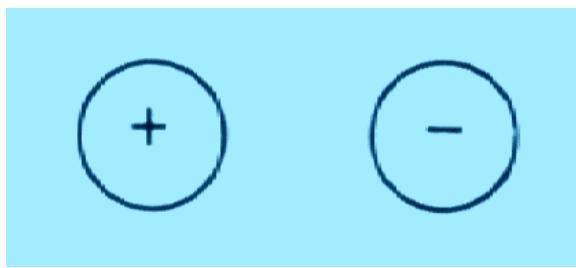
Možnosti překryvu orbitalů



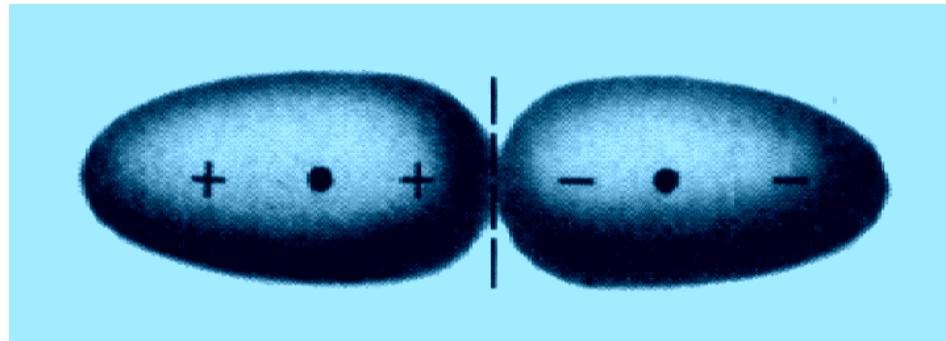
$s + s'$



σ_s



$s - s'$



σ_s^*

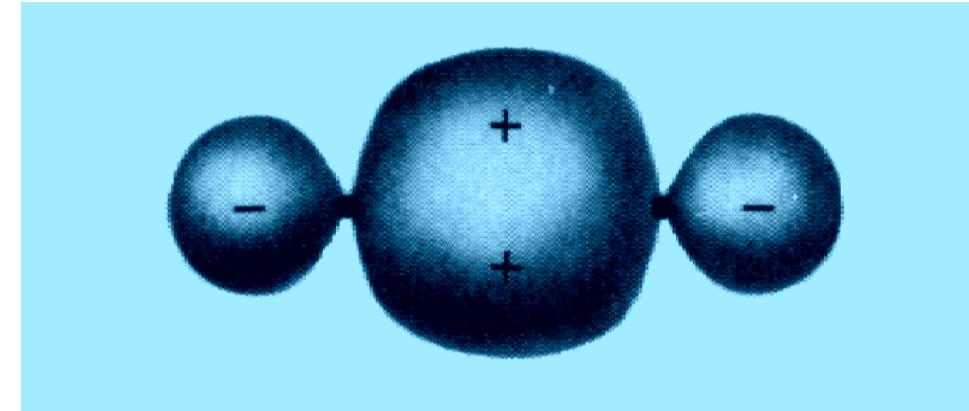
Možnosti překryvu orbitalů



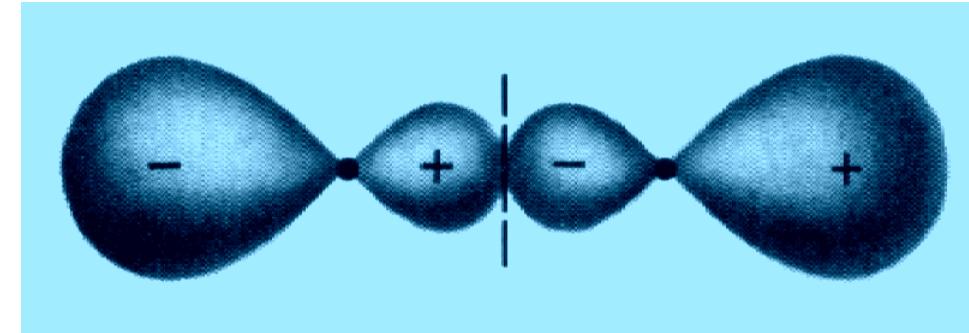
$$p_z + p_z'$$



$$p_z - p_z'$$

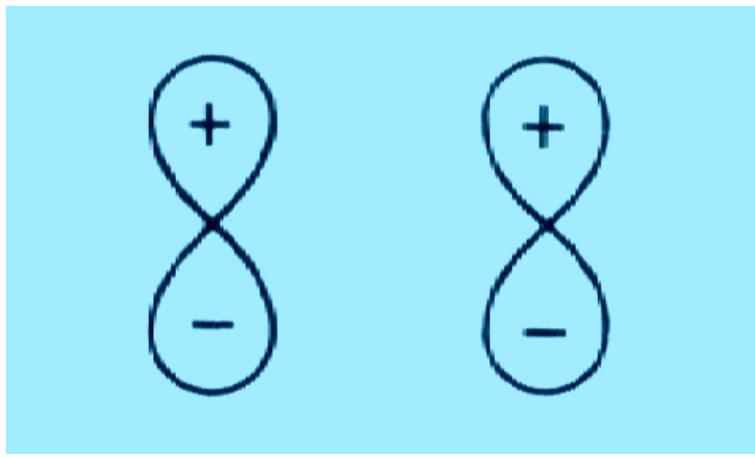


$$\sigma_p$$

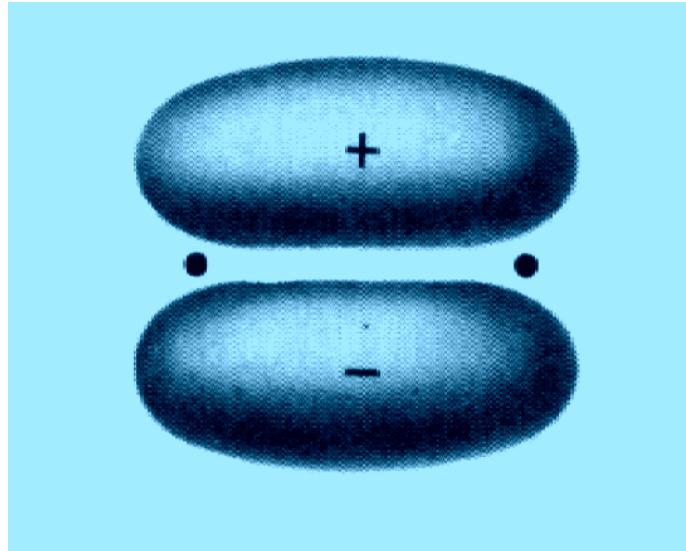


$$\sigma_p^*$$

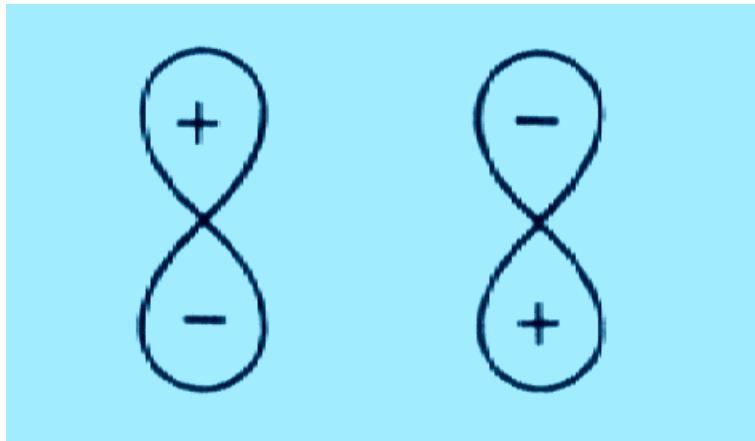
Možnosti překryvu orbitalů



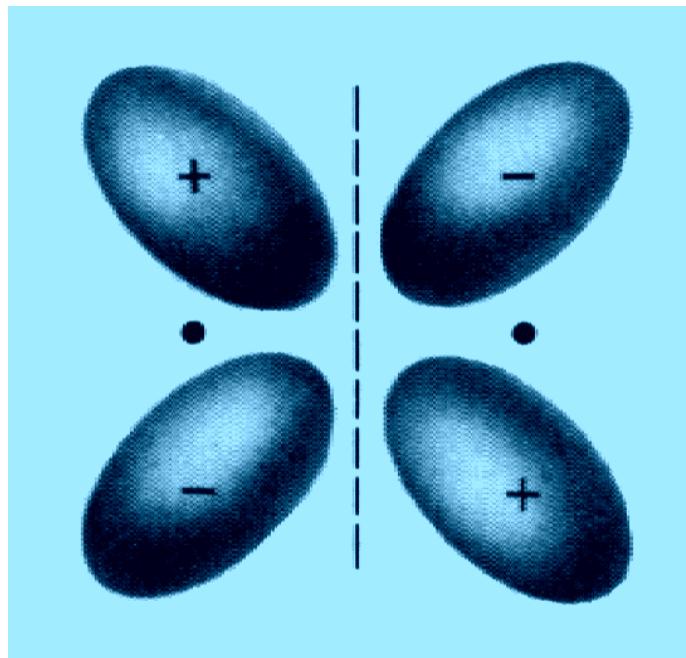
$p_x + p_x'$ nebo $p_y + p_y'$



π_x
nebo
 π_y

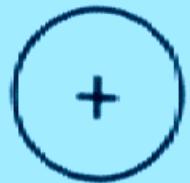


$p_x - p_x'$ nebo $p_y - p_y'$



π_x^*
nebo
 π_y^*

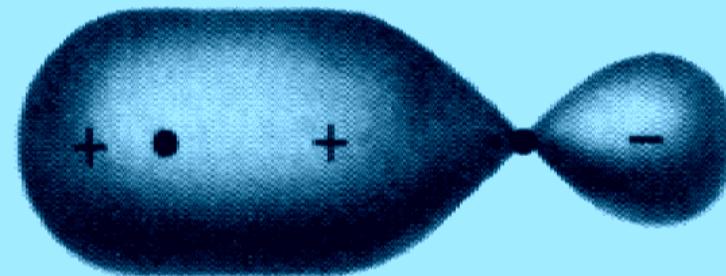
Možnosti překryvu orbitalů



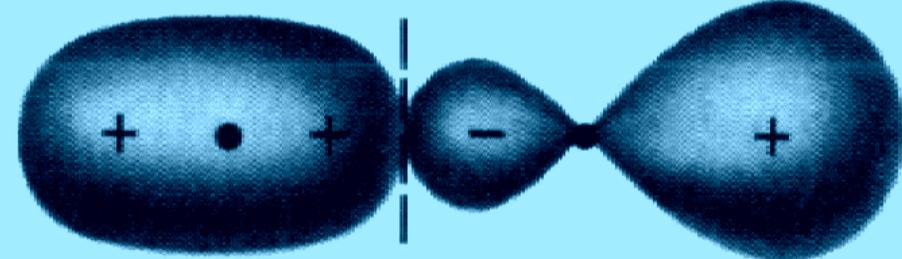
$s + p_z'$



$s - p_z'$

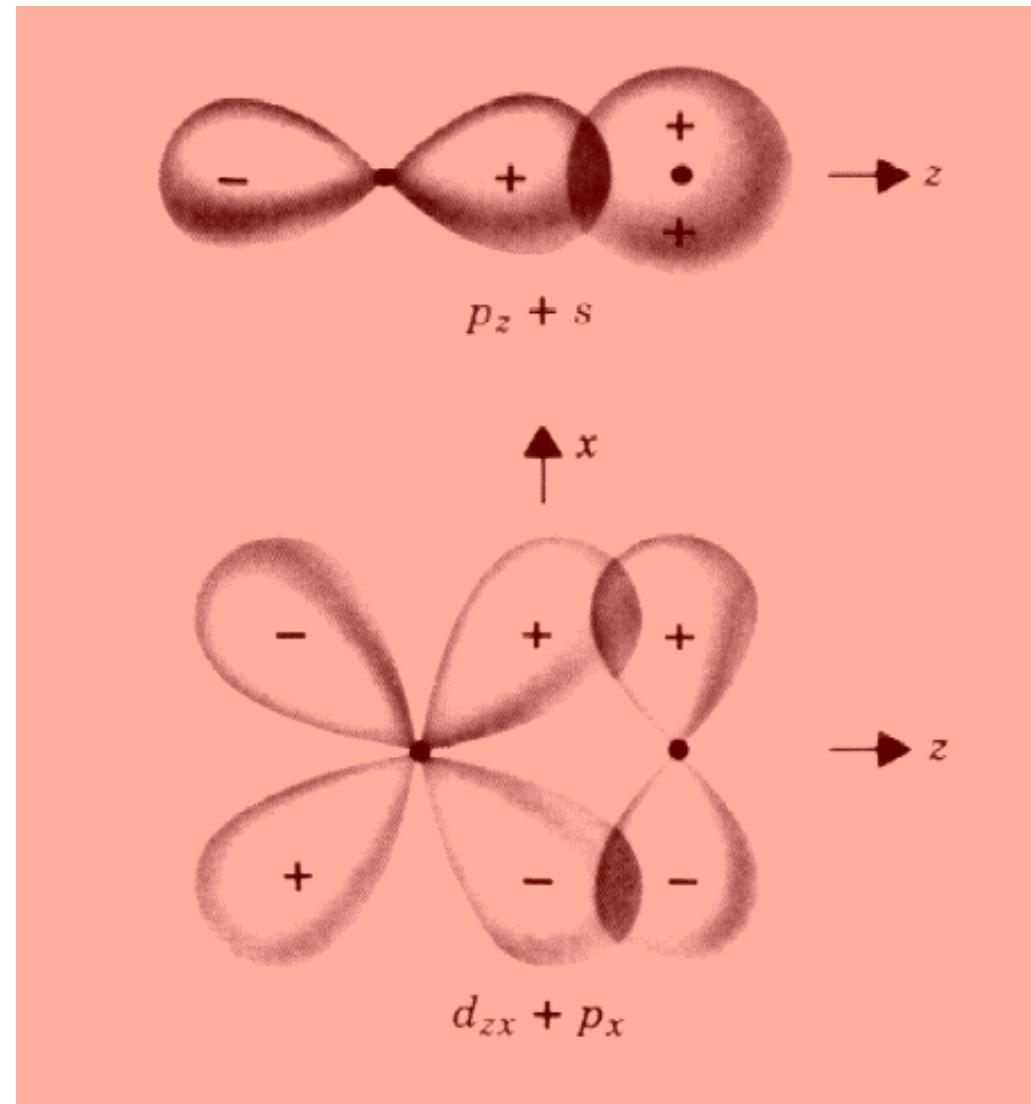
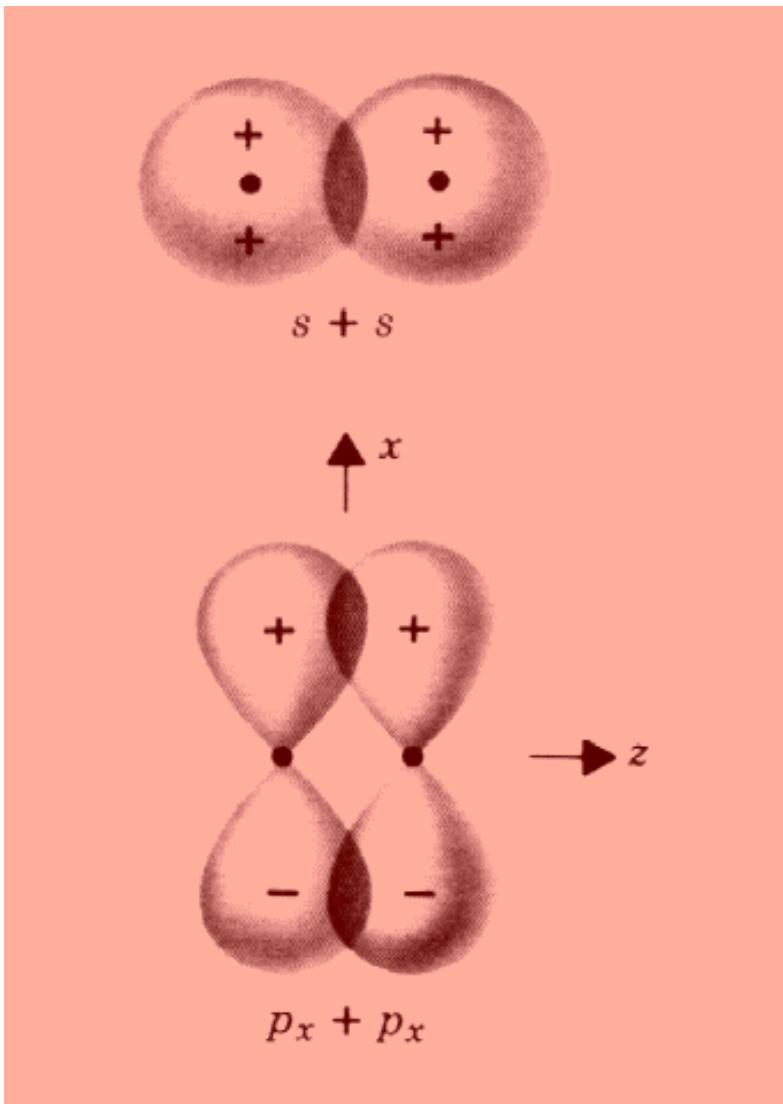


σ



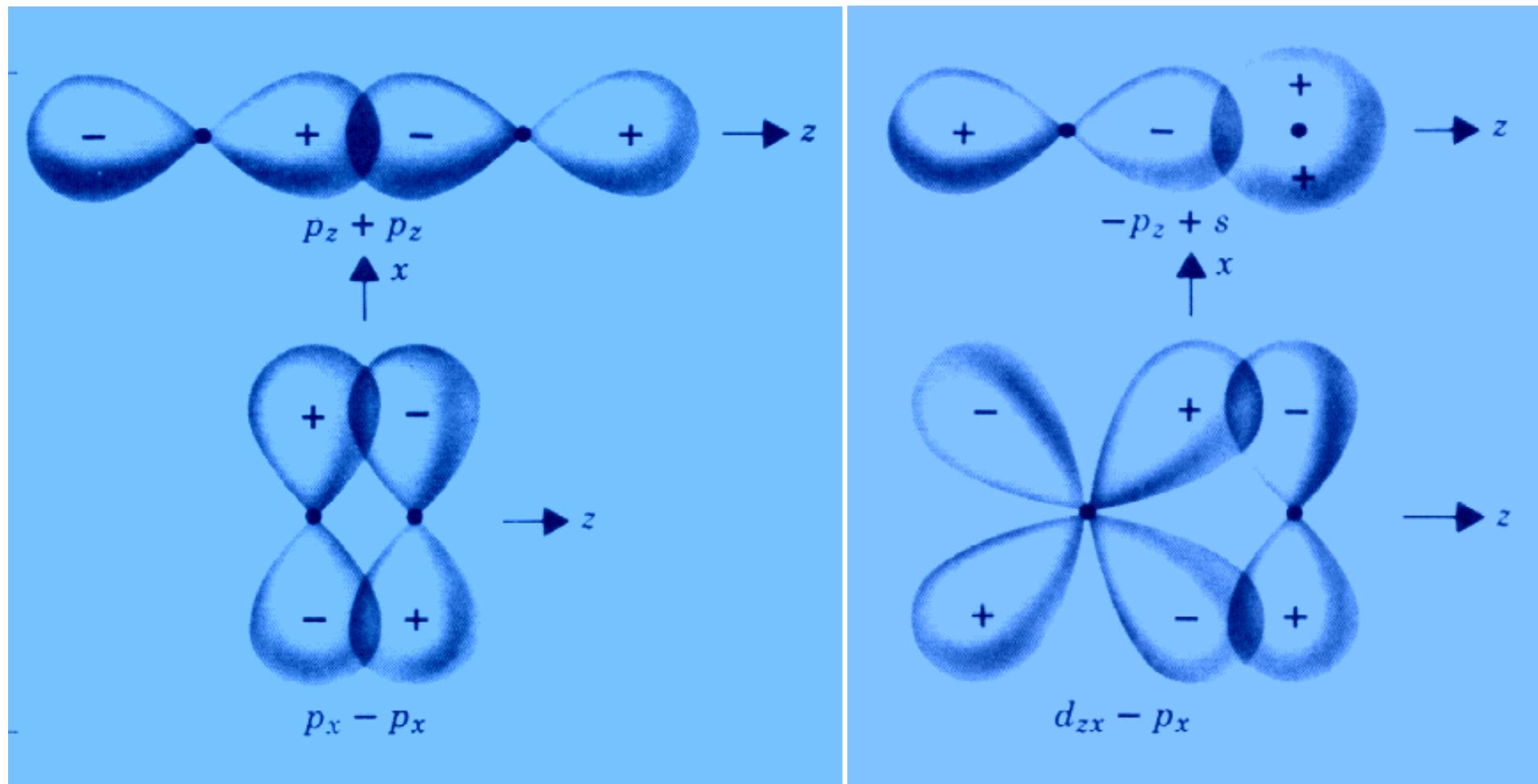
σ^*

Efektivita překryvu orbitalů



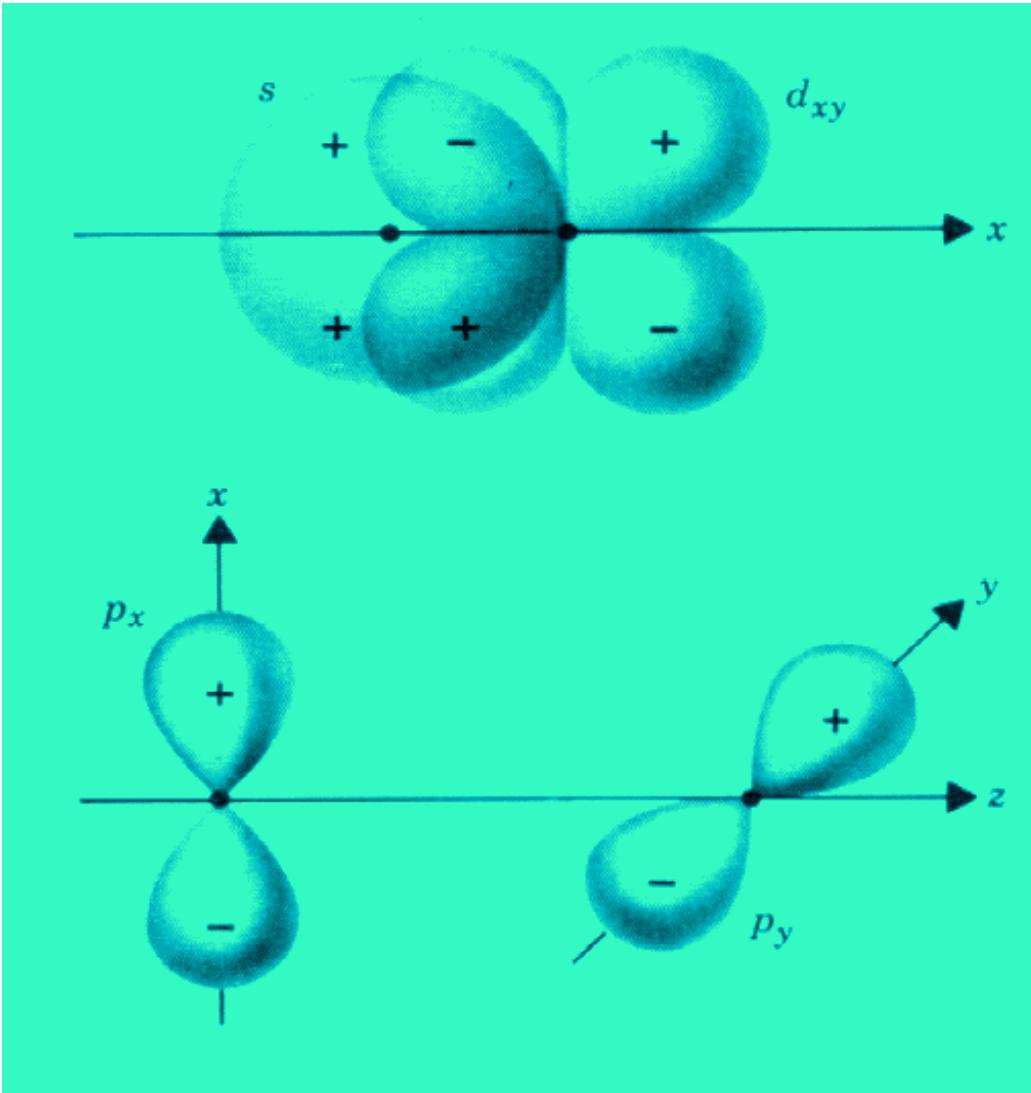
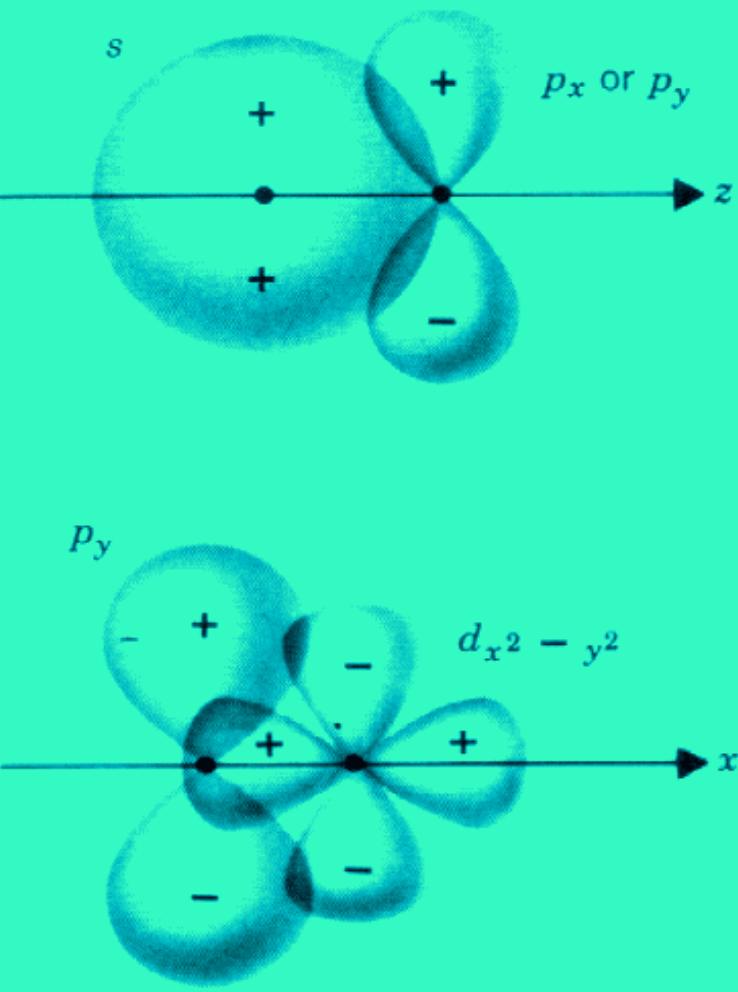
kladný (+) překryv – vazebný

Efektivita překryvu orbitalů



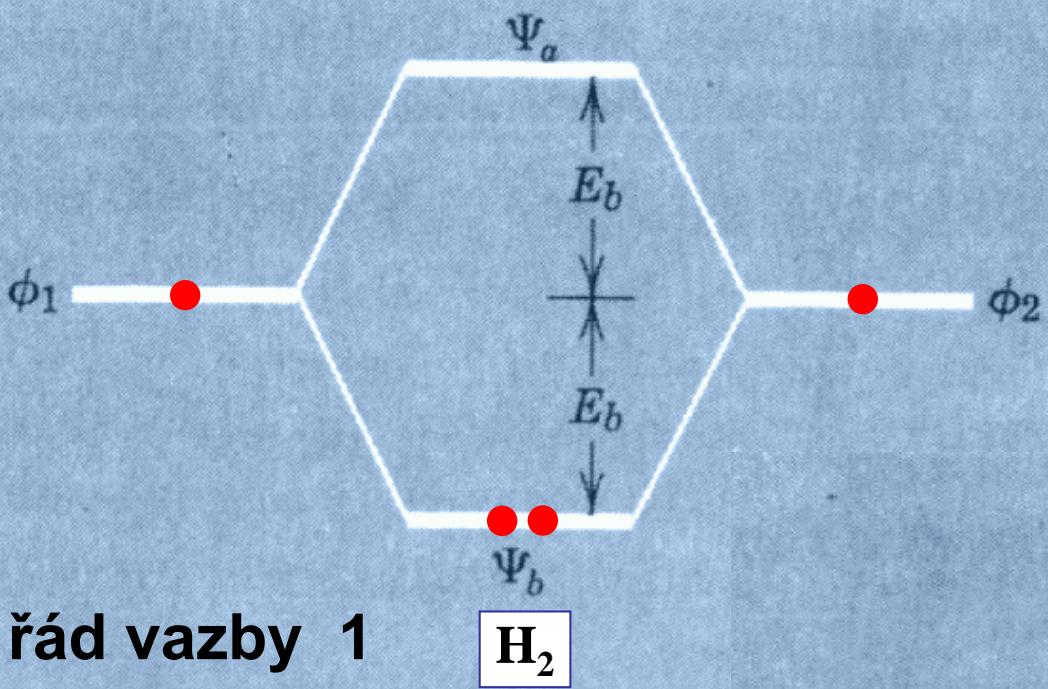
záporný **(-)** překryv – protivazebný

Efektivita překryvu orbitalů

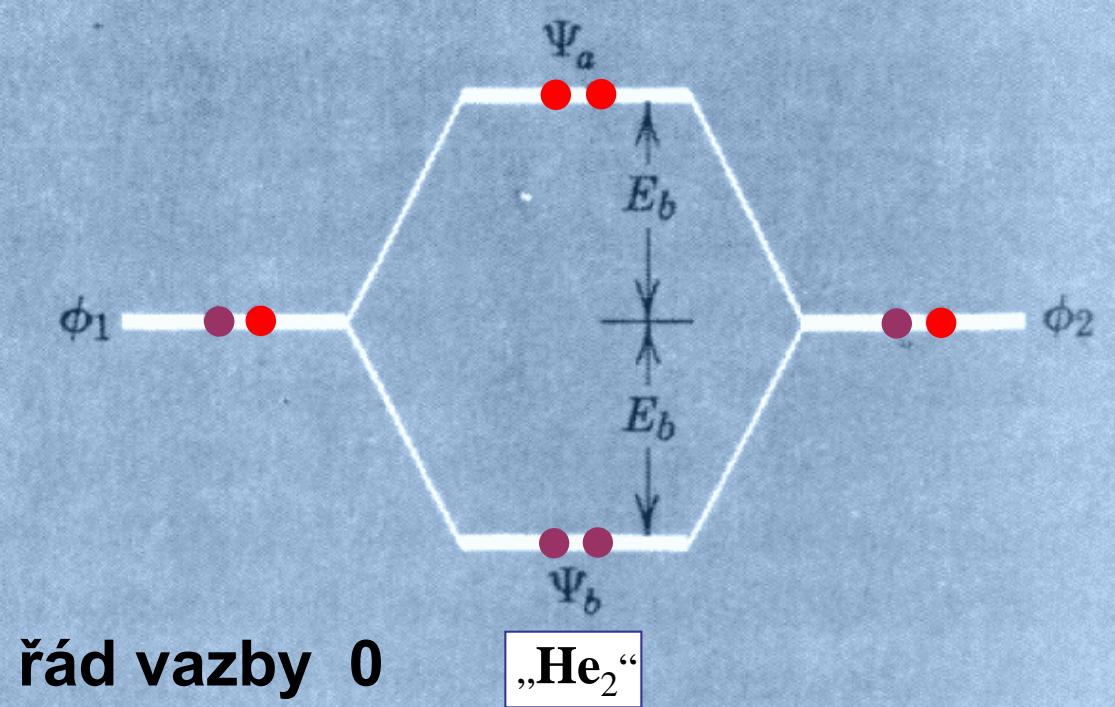


nulový (0) překryv – symetricky nedovolený

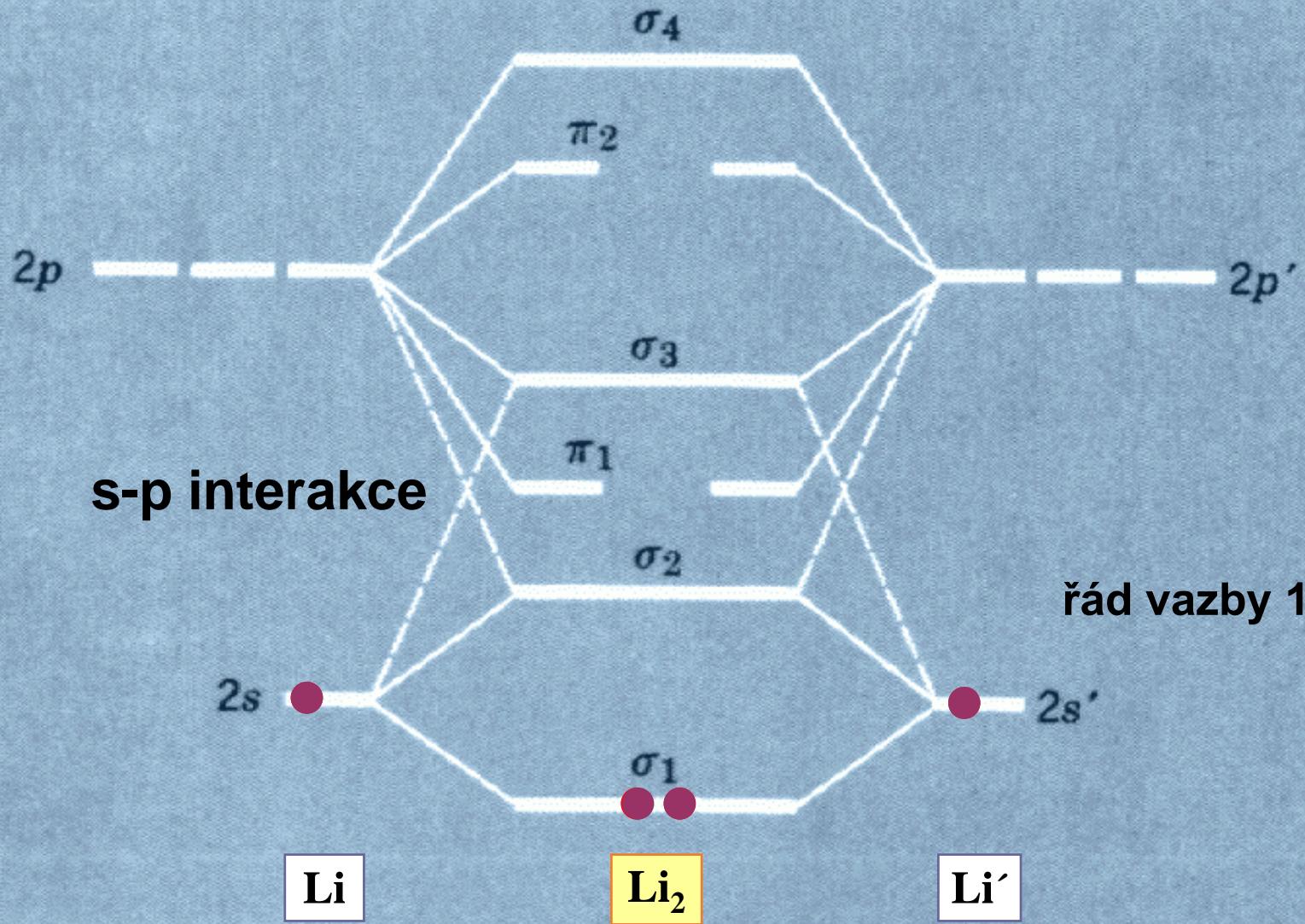
Molekulové orbitaly H_2 a „ He_2 “



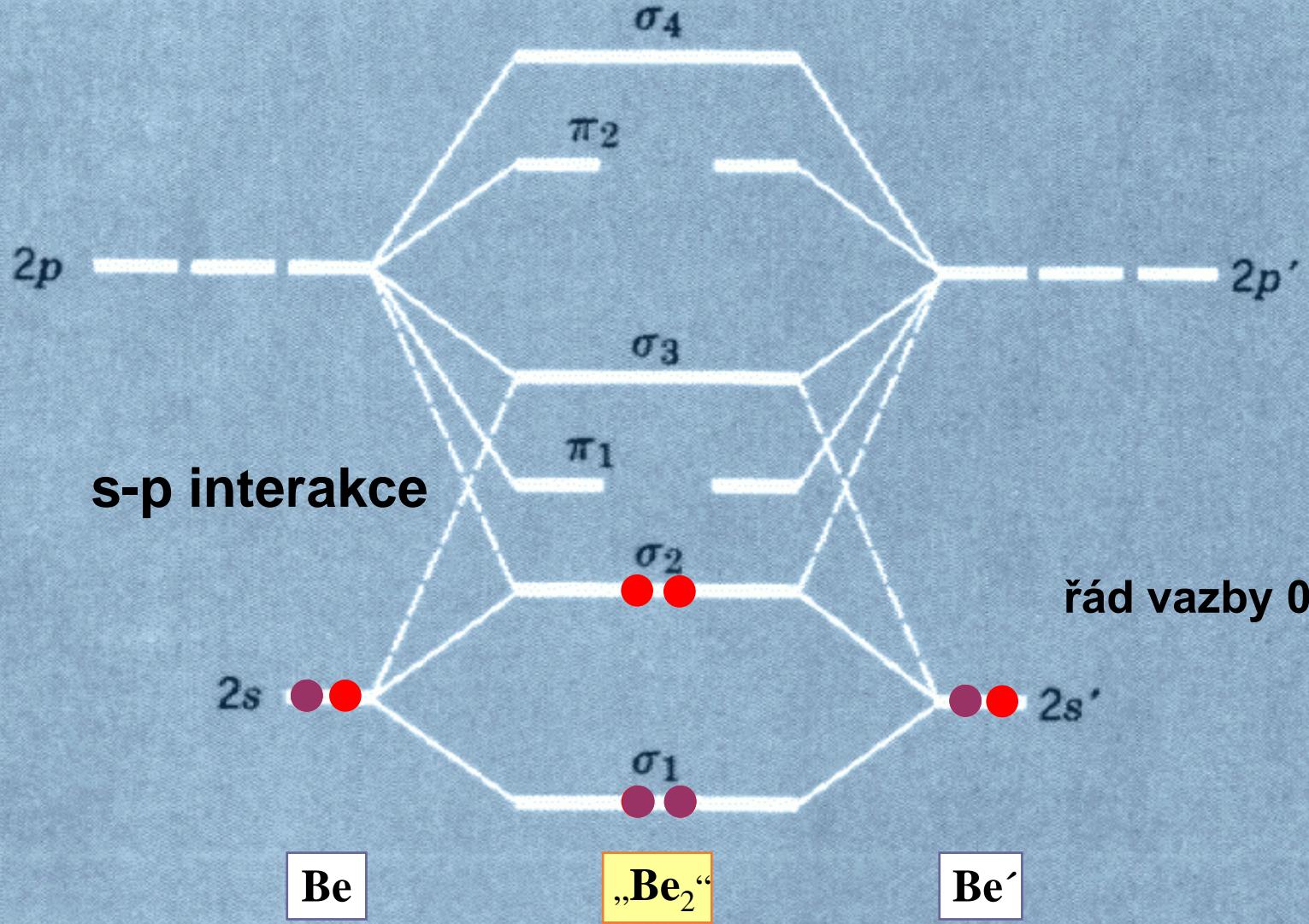
řad vazby:
 $n(e^- \text{ páru})_b - n(e^- \text{ páru})_a$
u diatomik
 $\frac{1}{2}[n(e^-)_b - n(e^-)_a]$



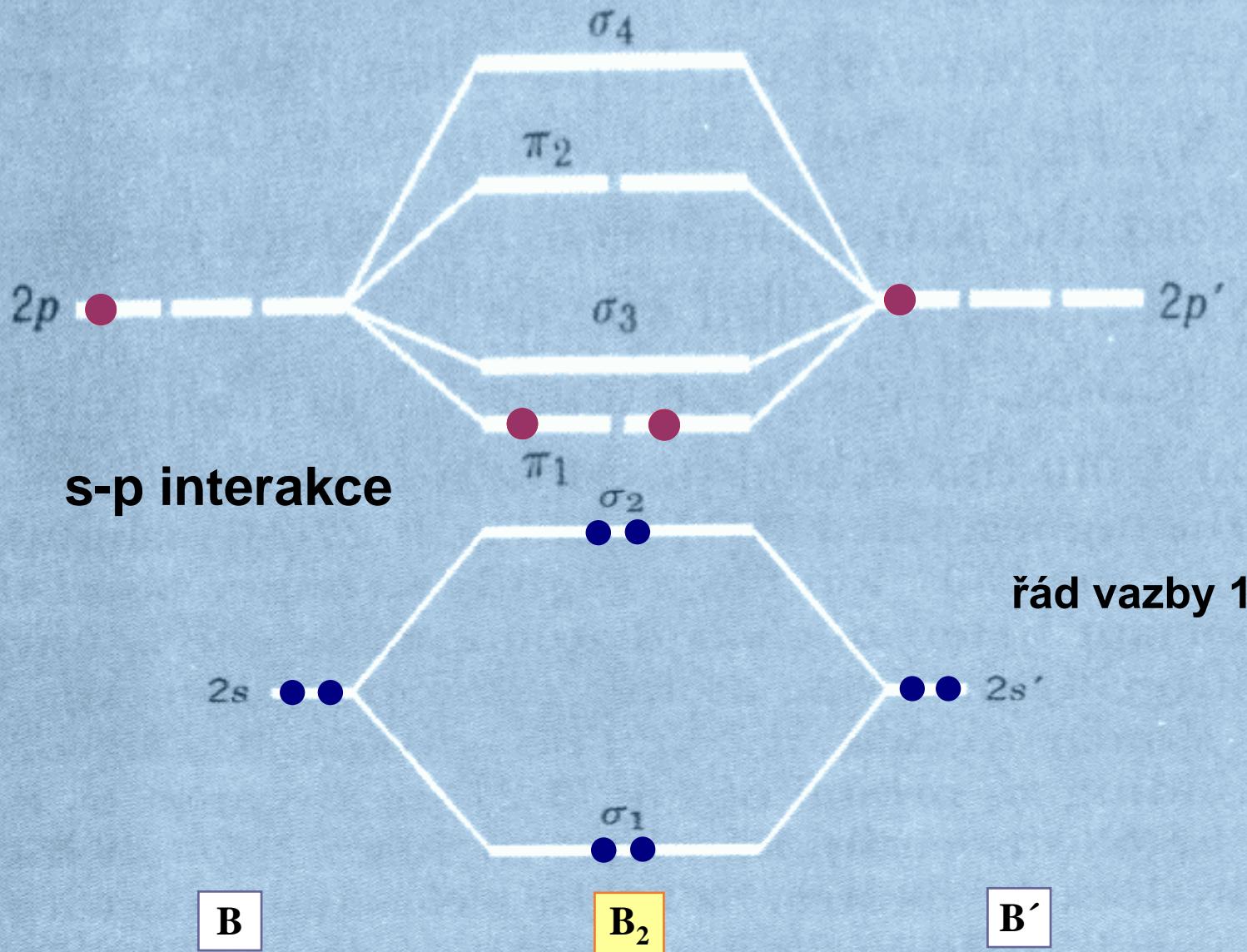
Molekulové orbitaly Li_2



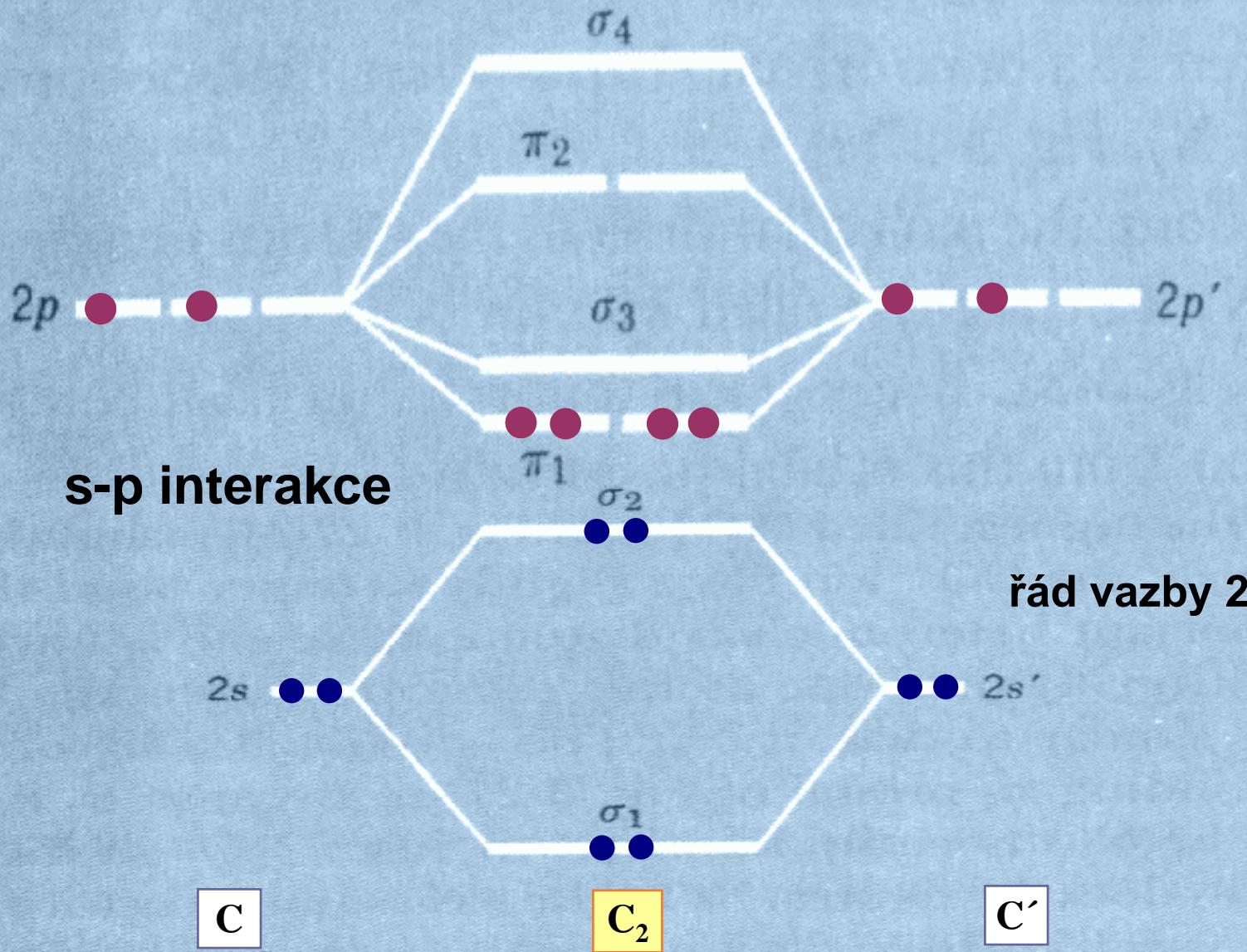
Molekulové orbitaly „Be₂“



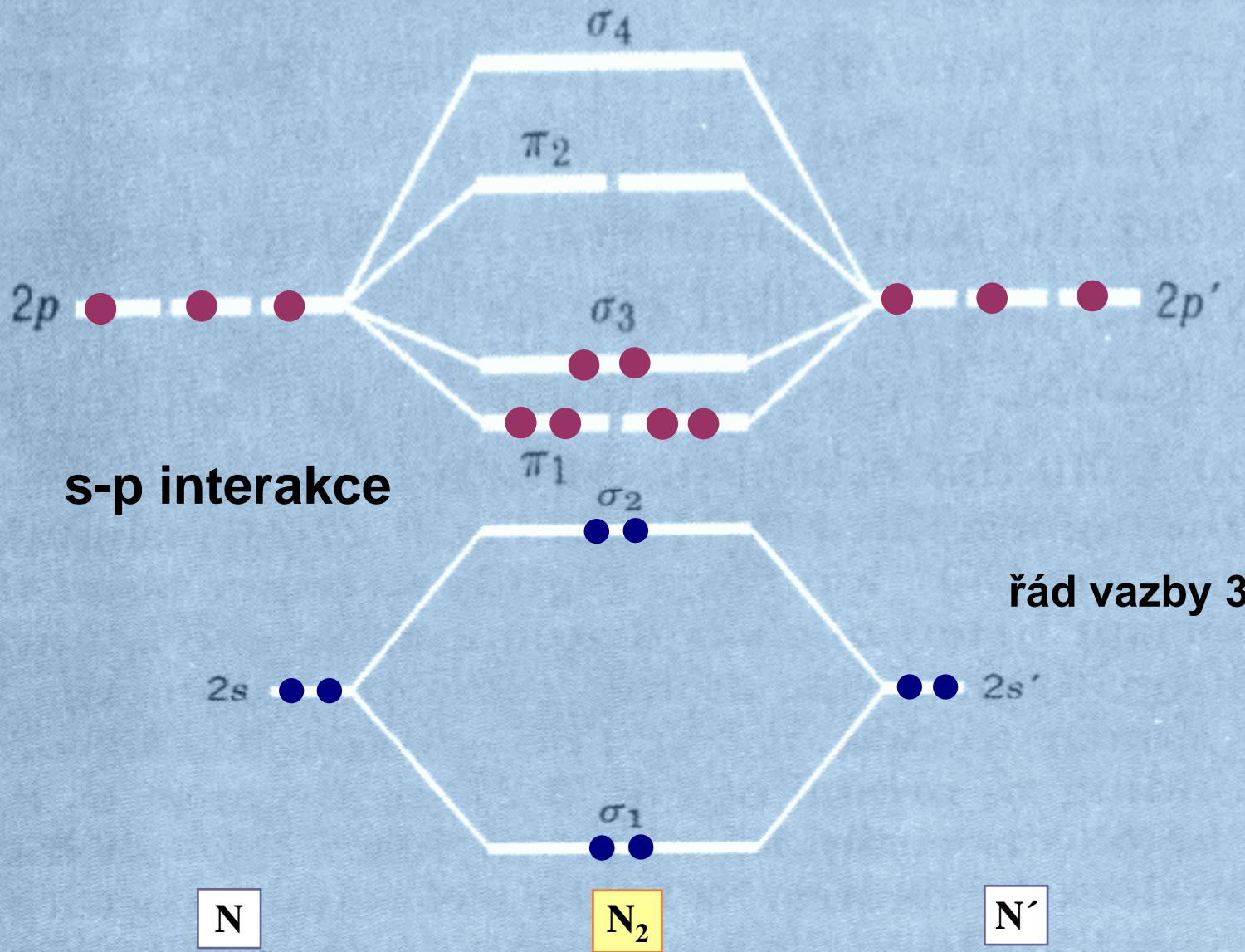
Molekulové orbitaly B_2



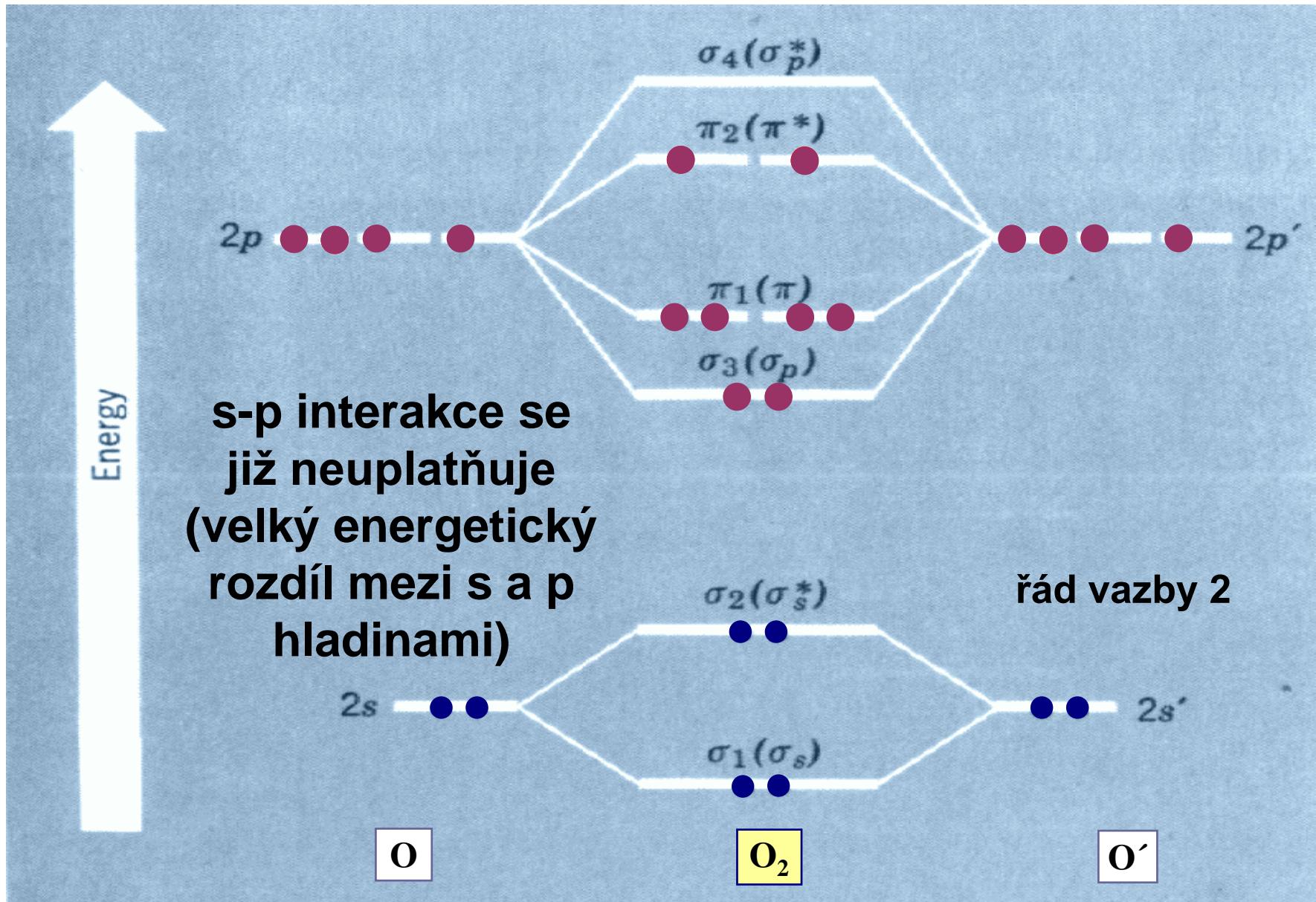
Molekulové orbitaly C_2



Molekulové orbitaly N_2

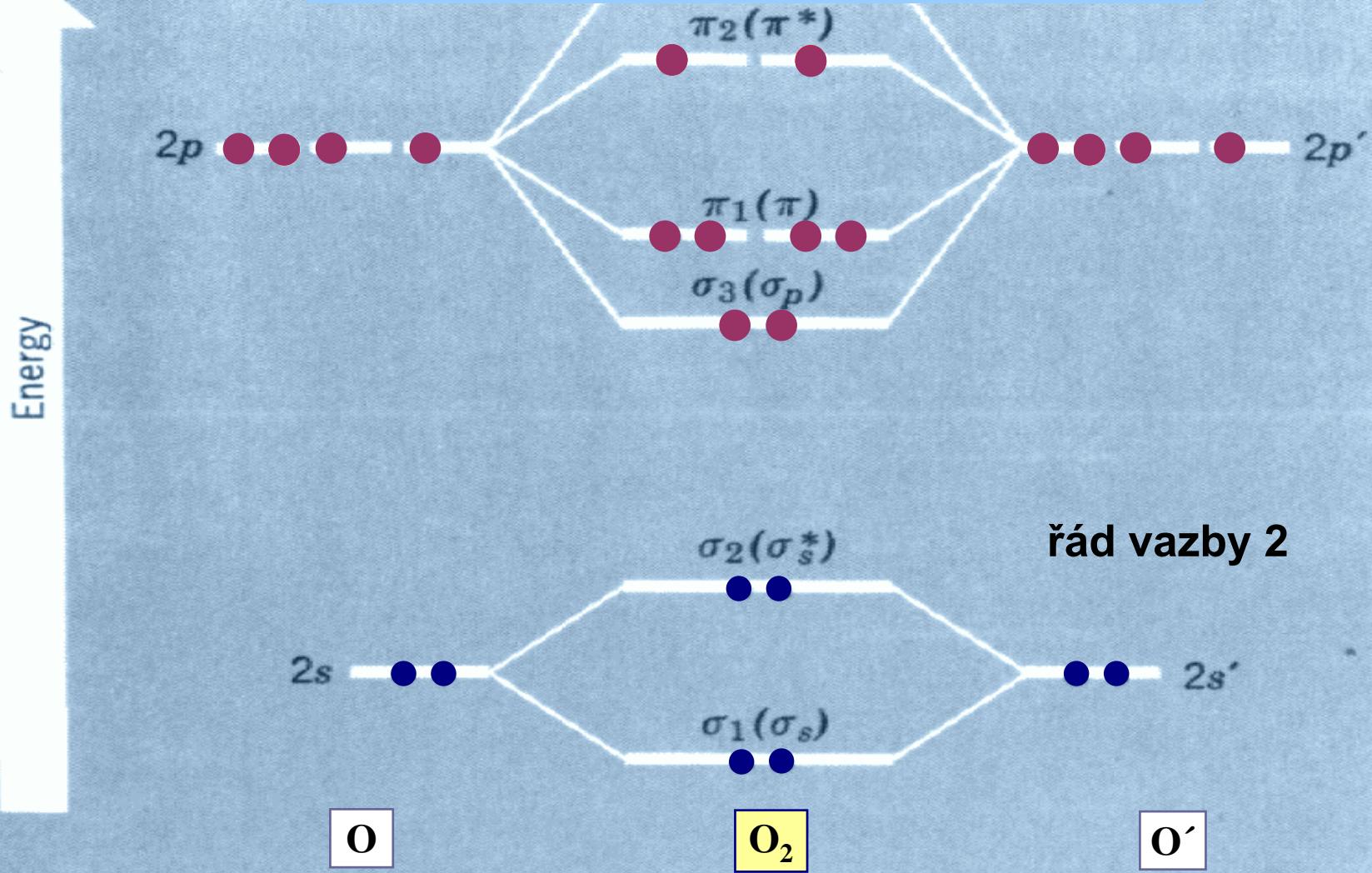


Molekulové orbitaly O_2

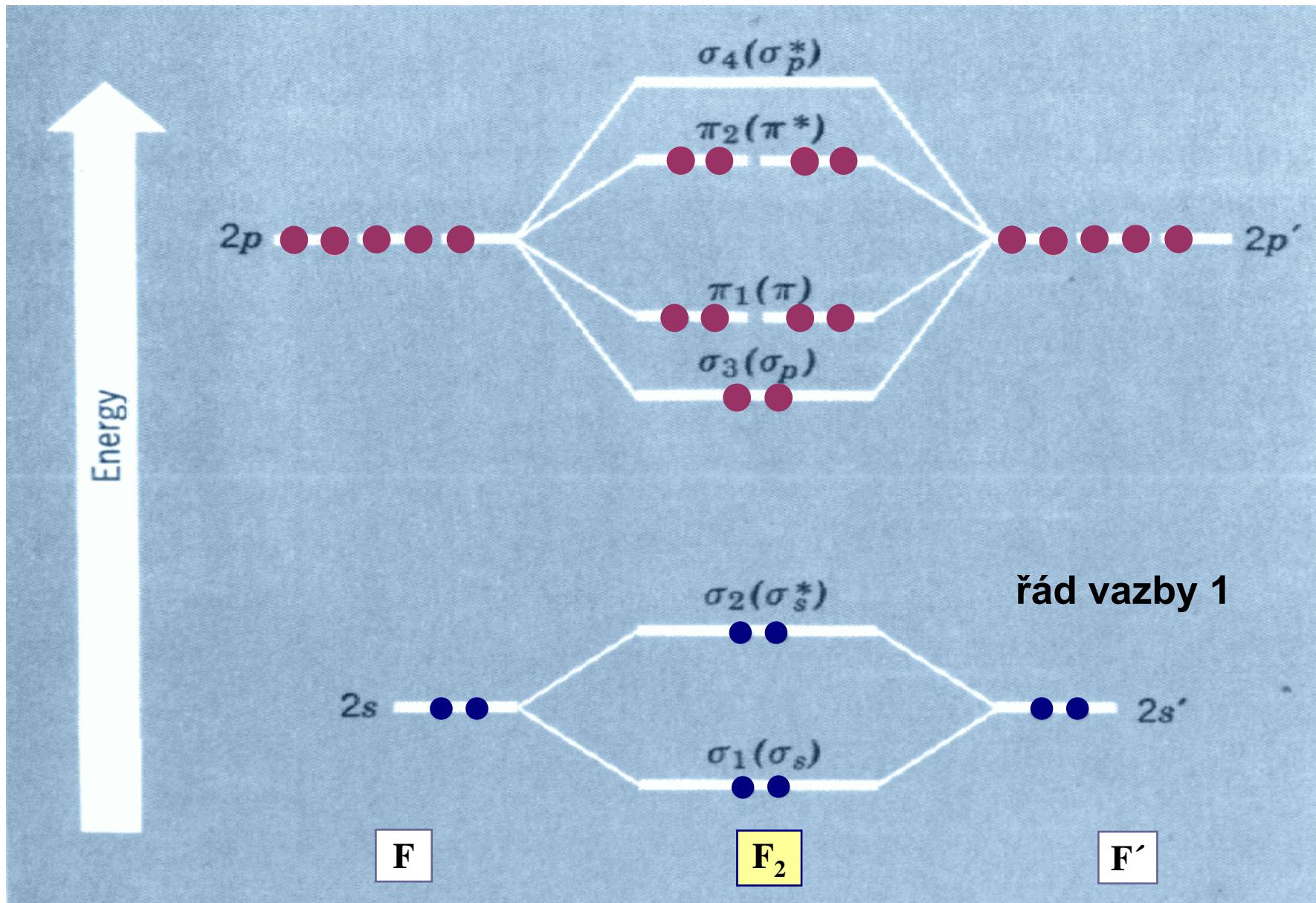


Molekulové orbitaly O₂

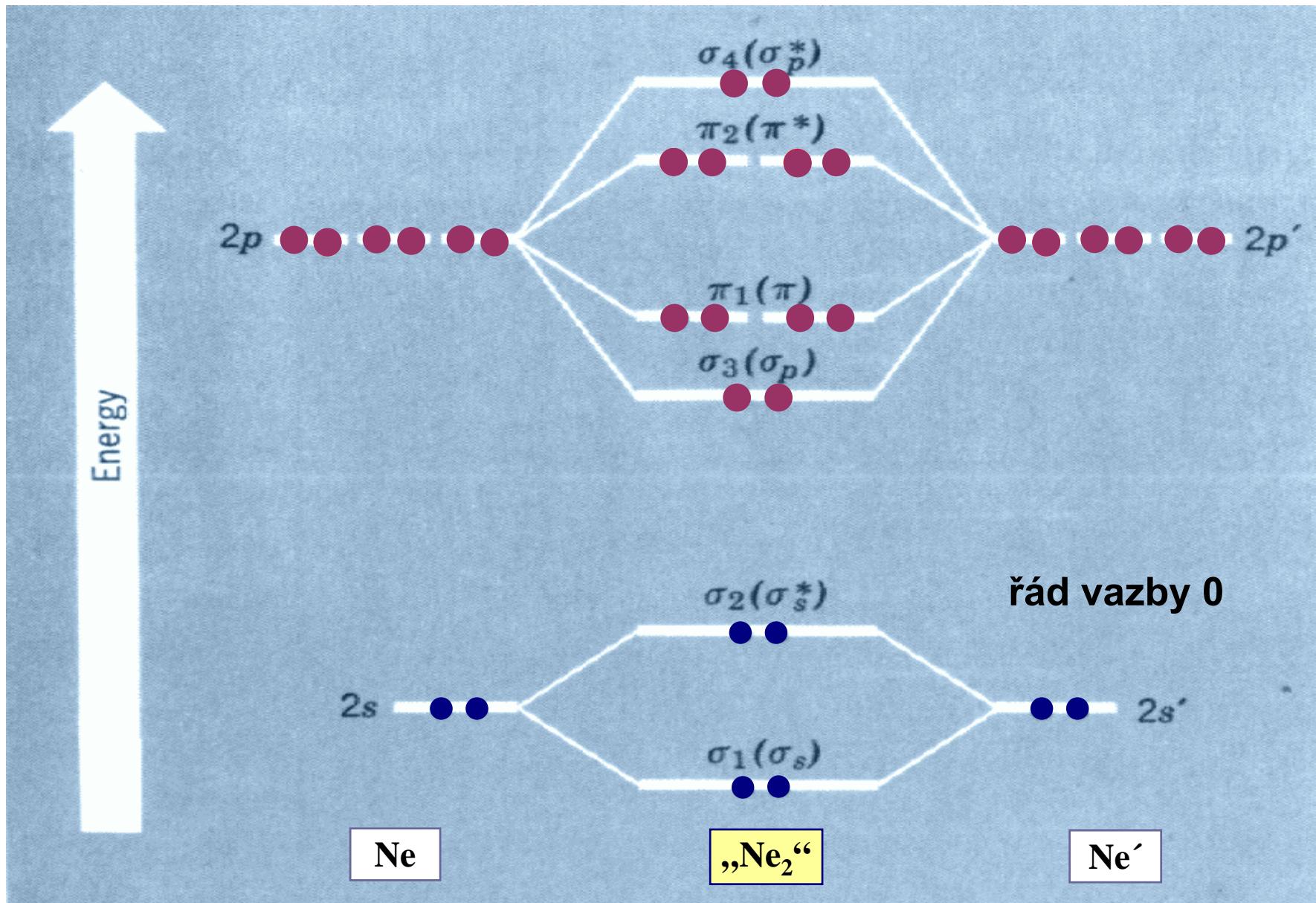
kyslík je diradikál – triplet

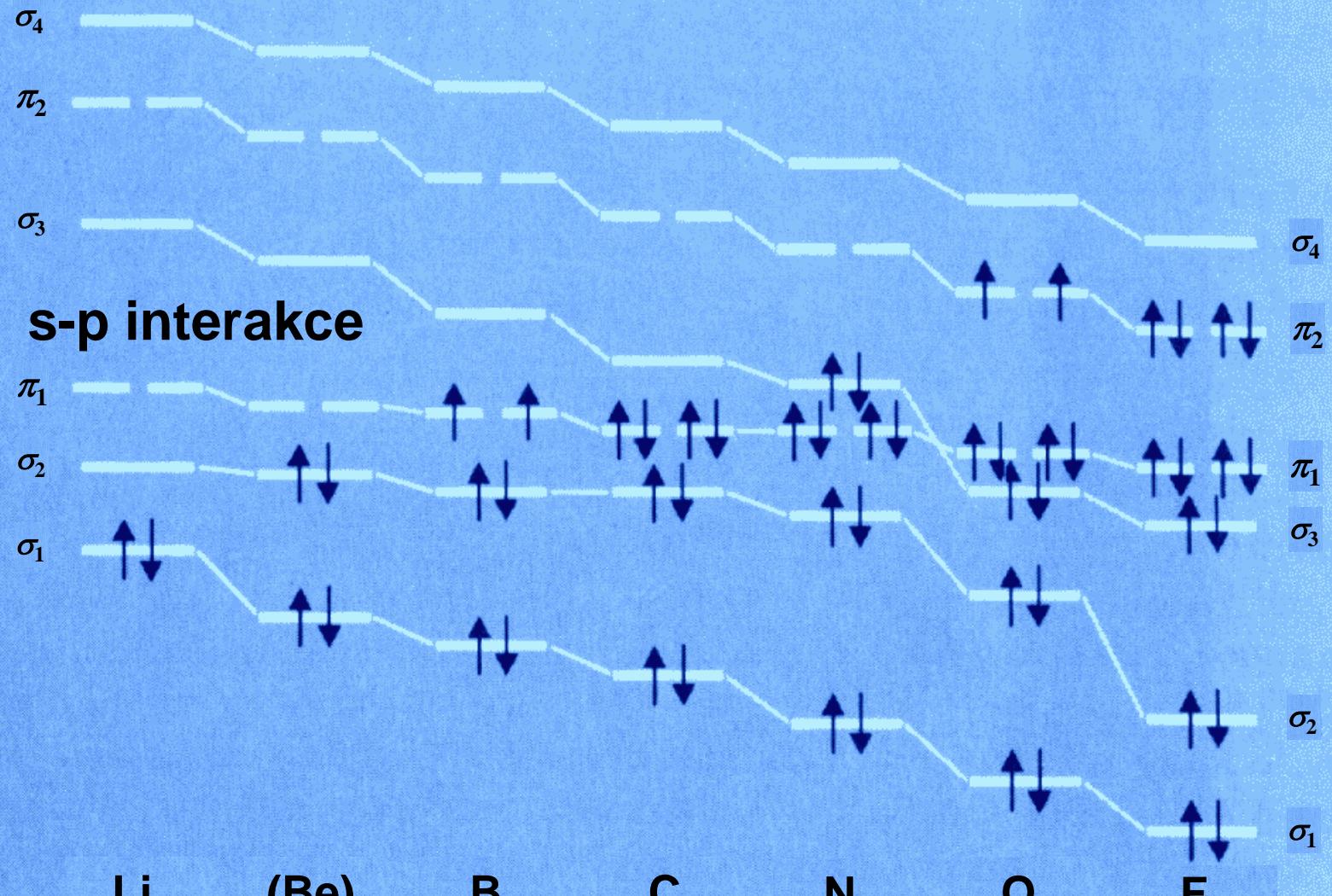


Molekulové orbitaly F_2



Molekulové orbitaly „Ne₂“





Li_2

$(\text{Be})_2$

B_2

C_2

N_2

O_2

F_2

Délka vazby (Å)

2,67

–

1,59

1,24

1,10

1,21

1,42

Vazebná energie (kJ.mol⁻¹)

110

–

272

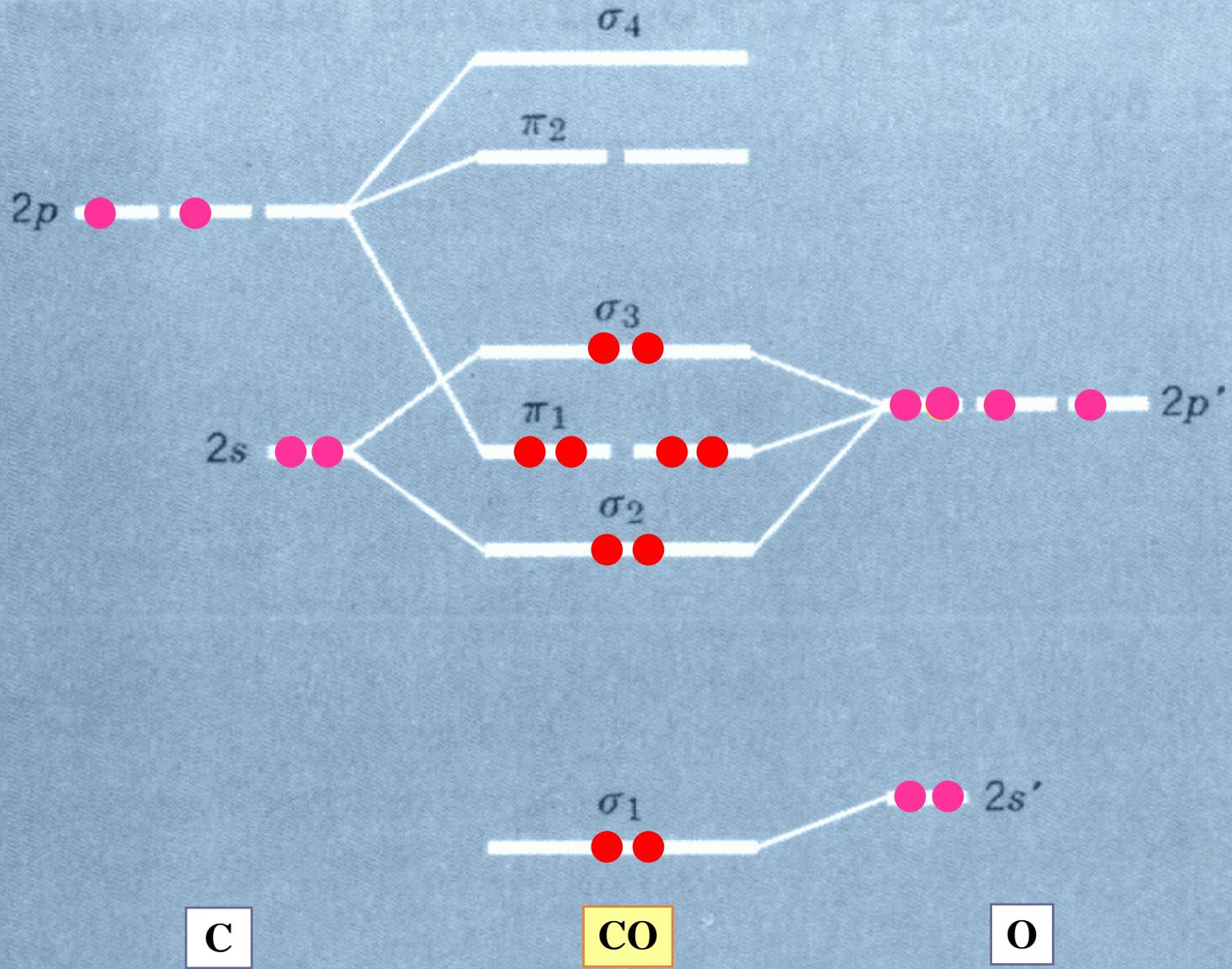
602

941

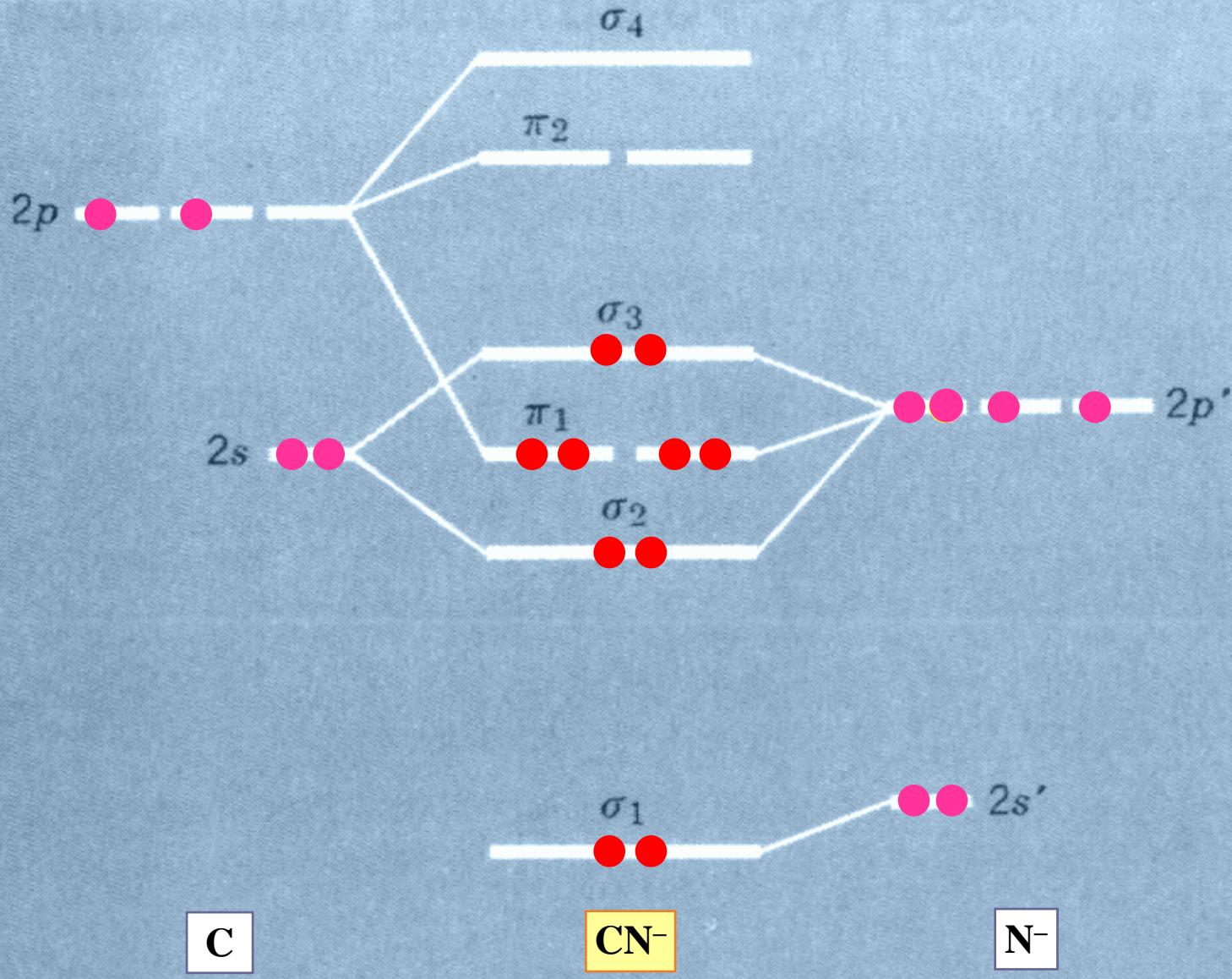
493

138

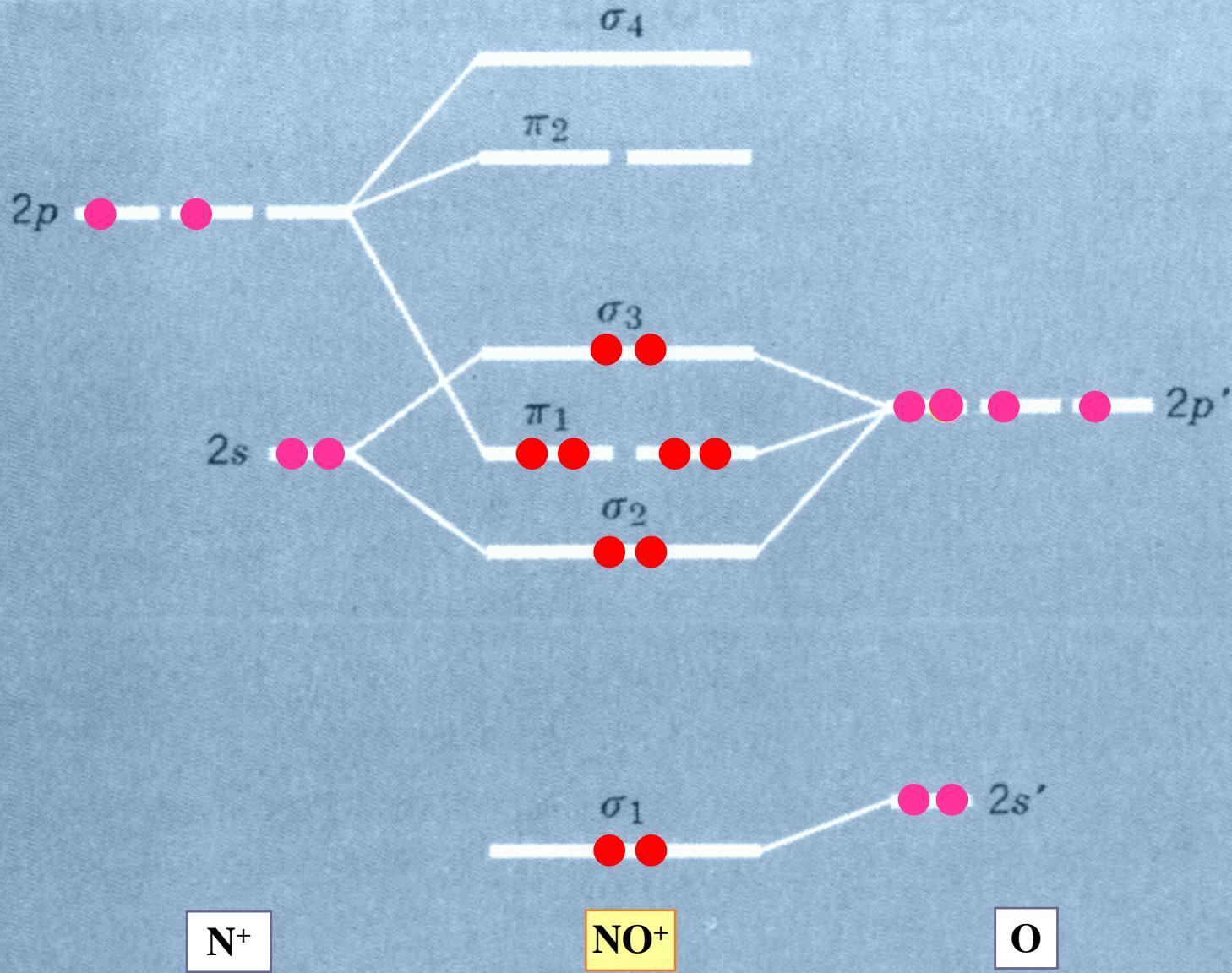
Molekulové orbitaly CO



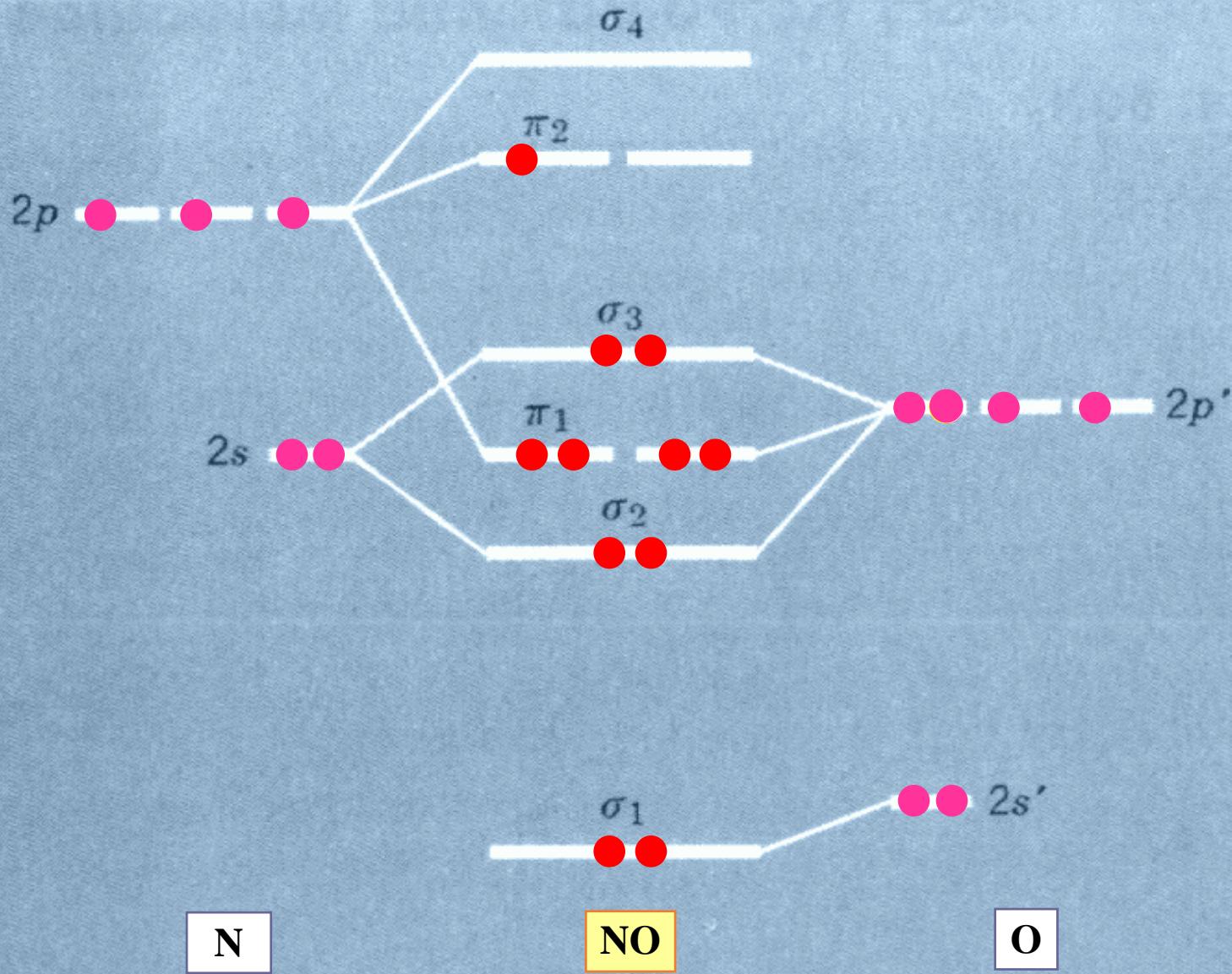
Molekulové orbitaly CN^-



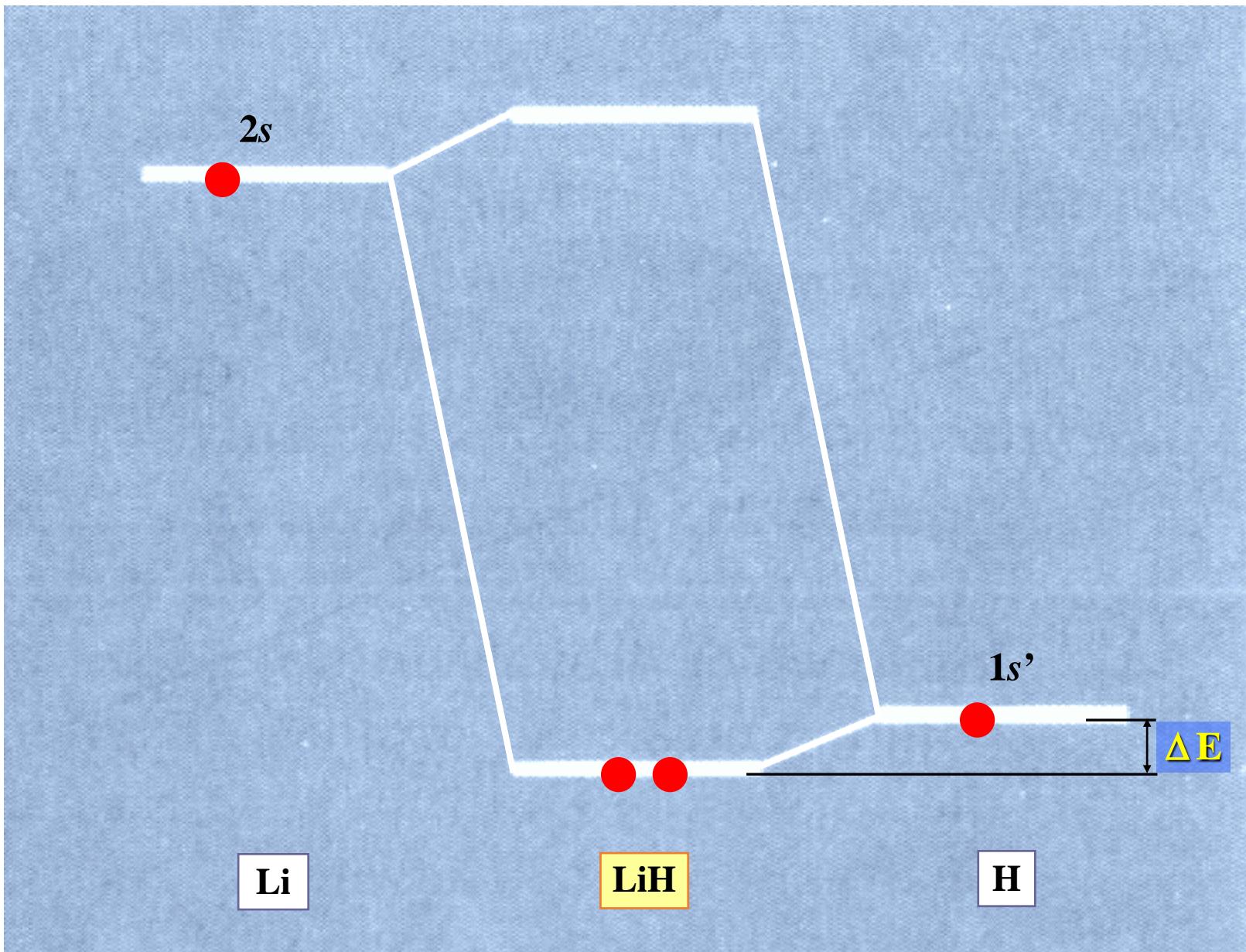
Molekulové orbitaly NO^+



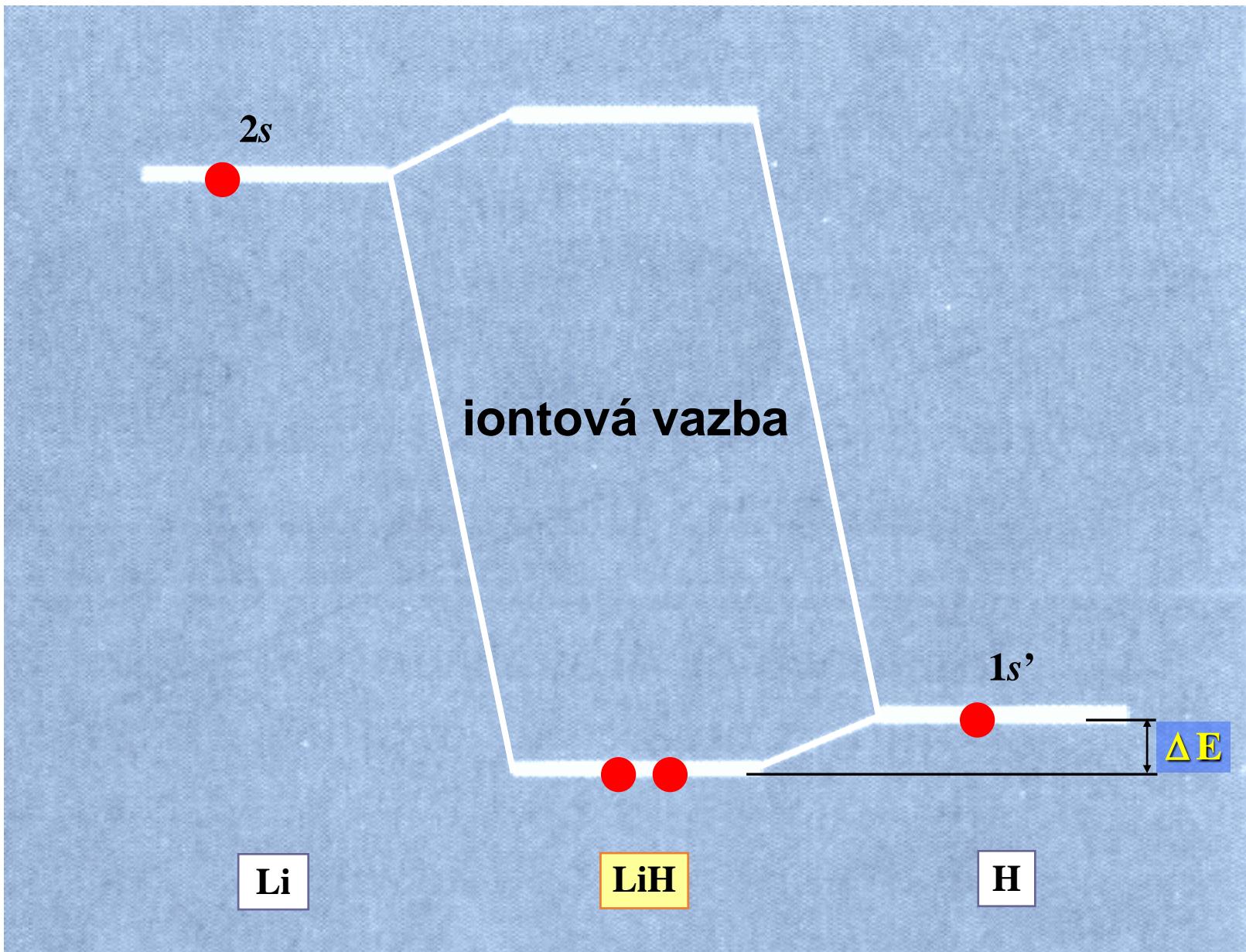
Molekulové orbitaly NO



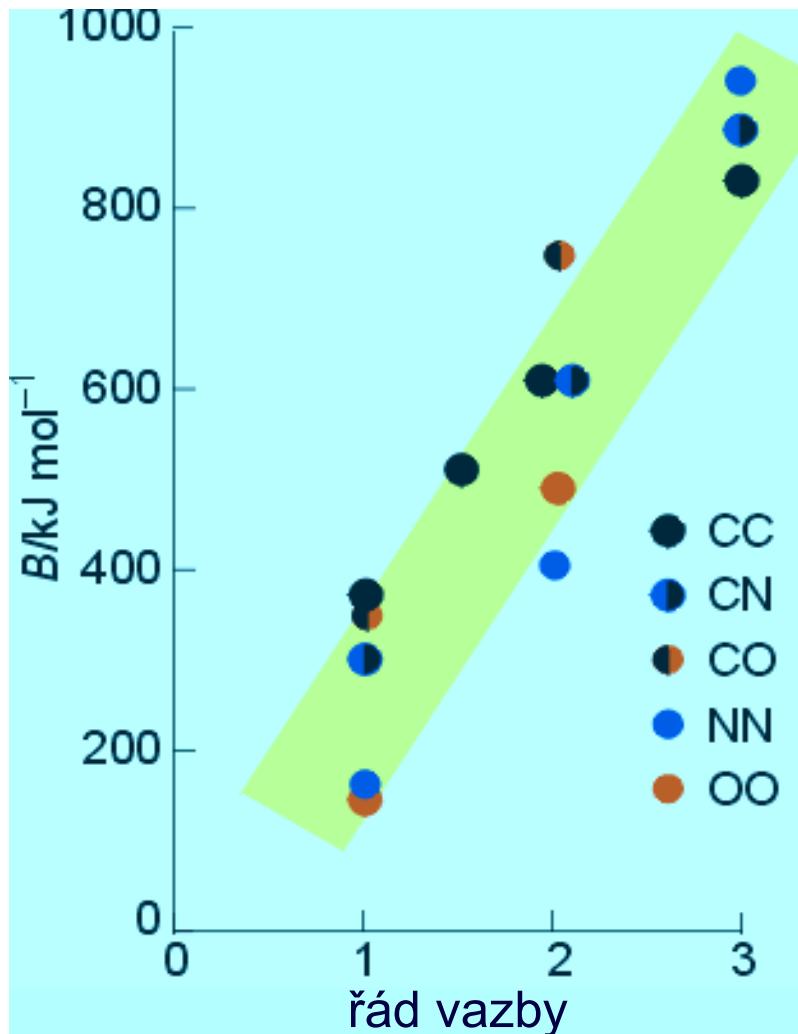
Molekulové orbitaly LiH



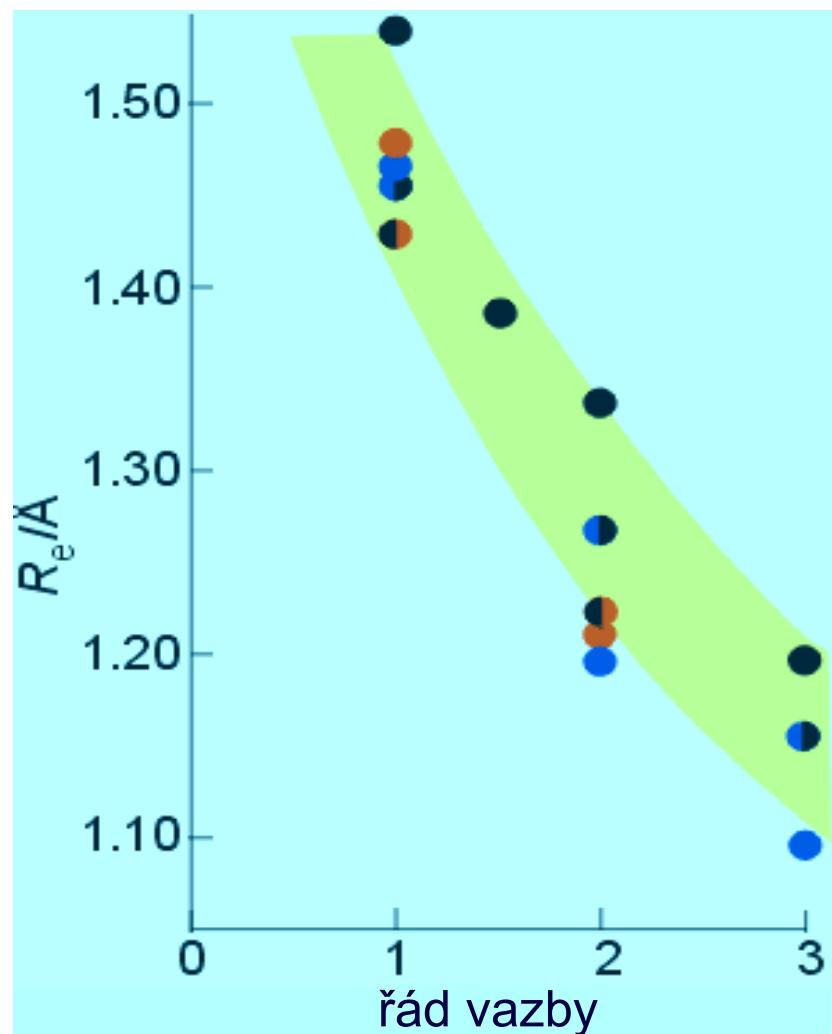
Molekulové orbitaly LiH



Korelace řádu vazby

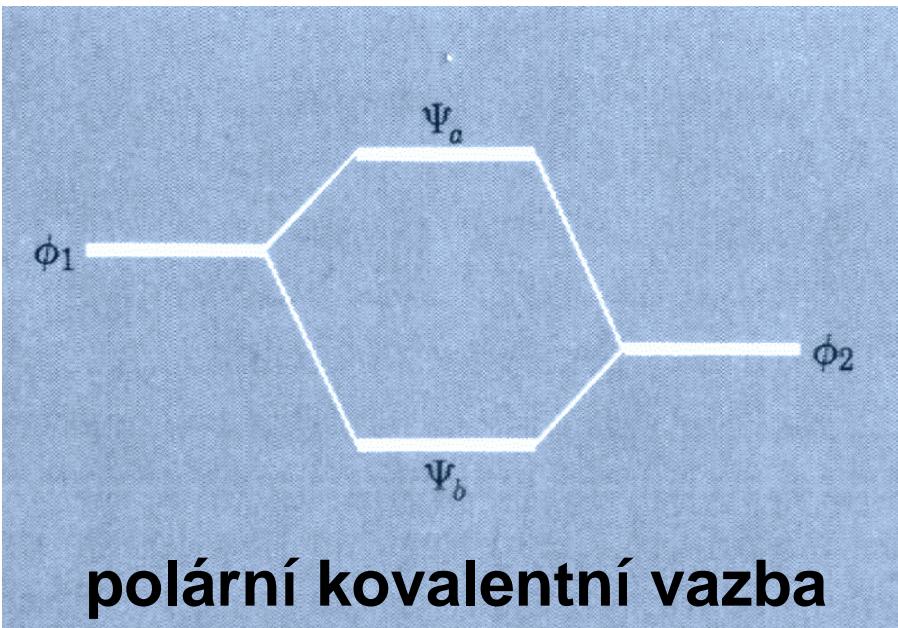
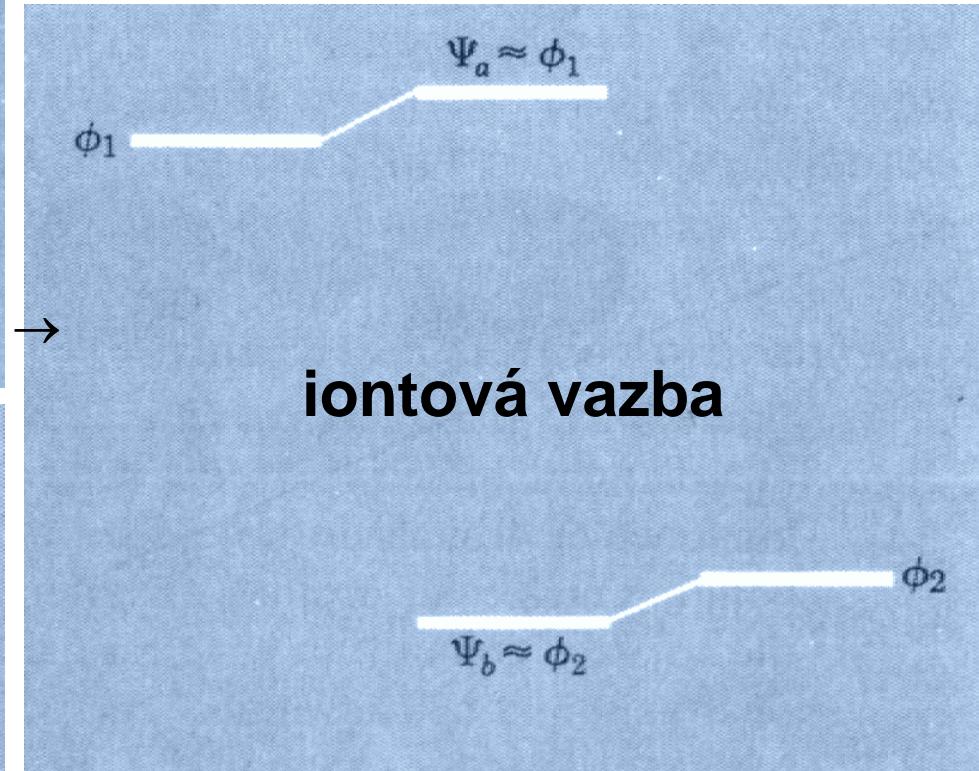
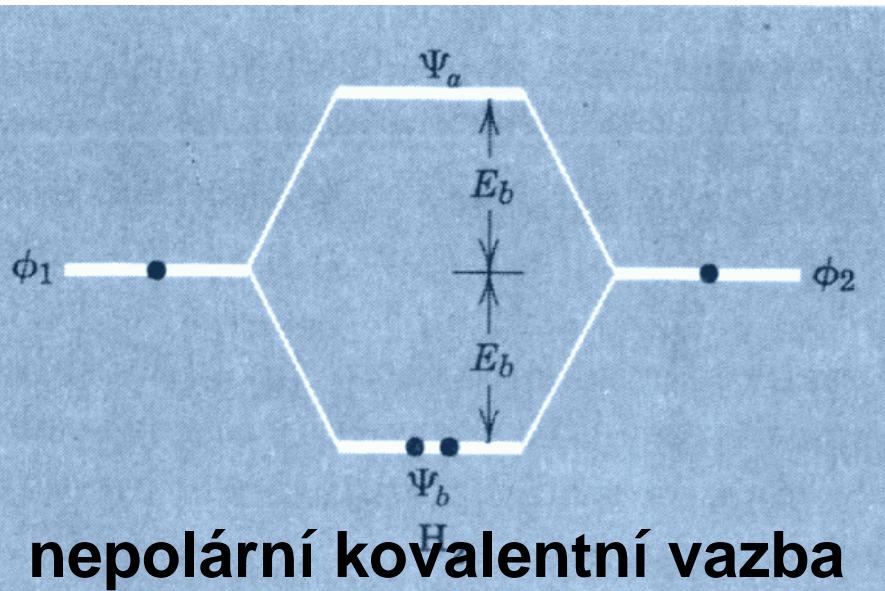


korelace
síly a řádu vazby

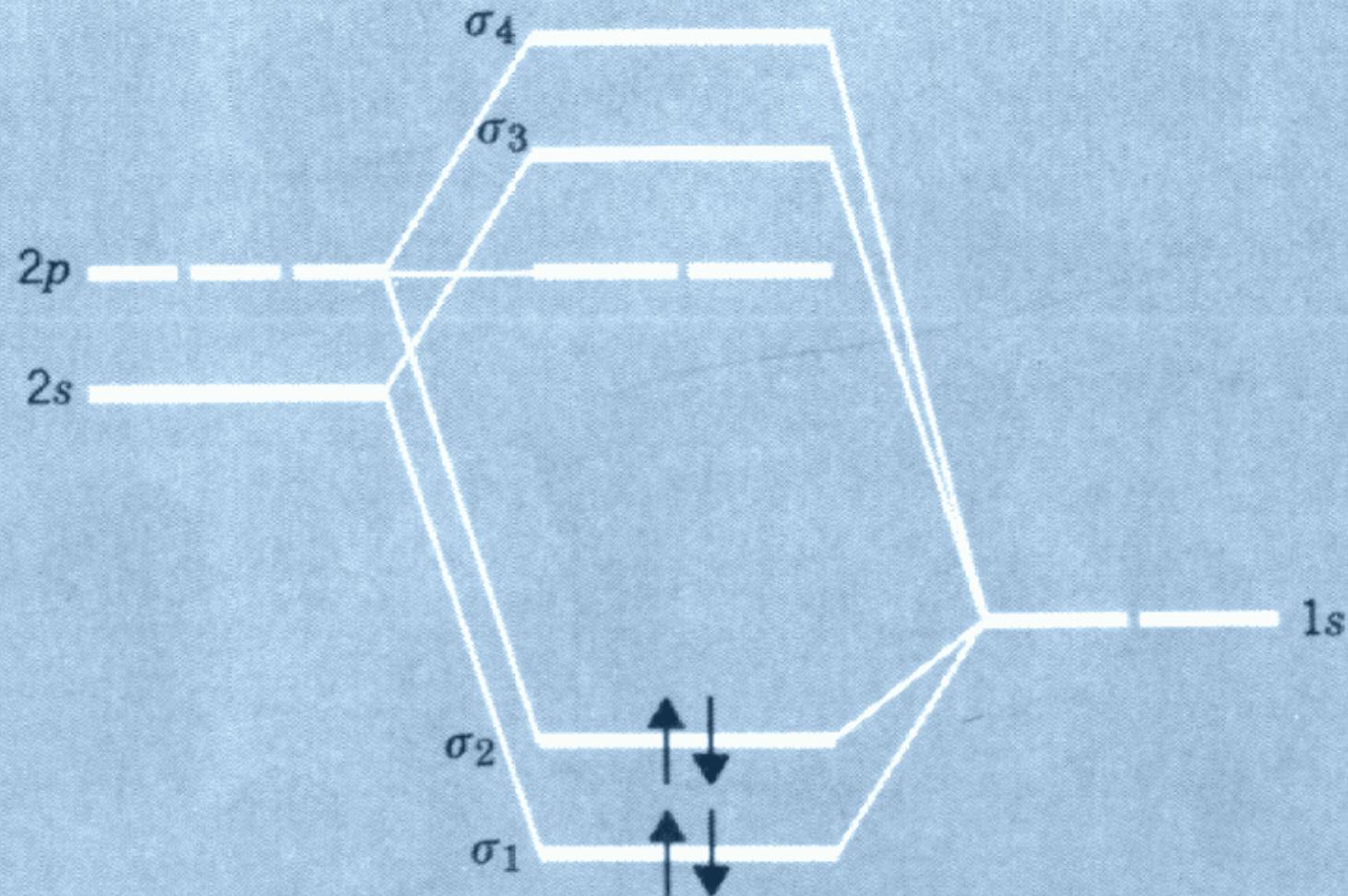


korelace
délky a řádu vazby

Polarita vazeb



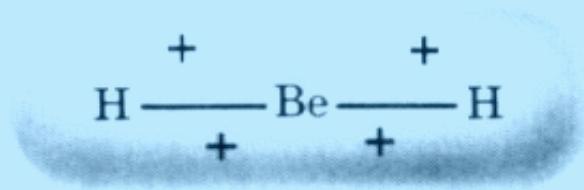
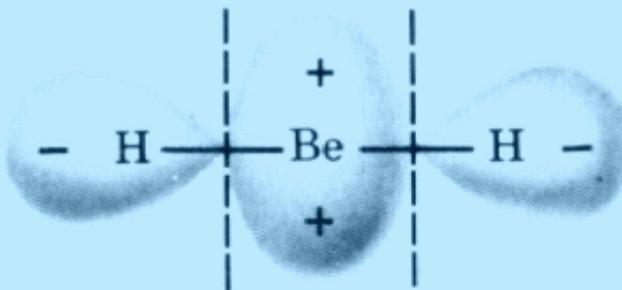
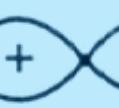
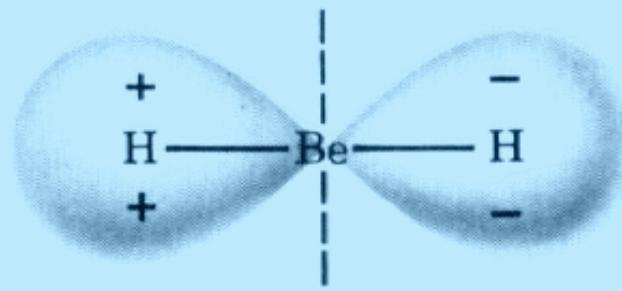
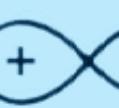
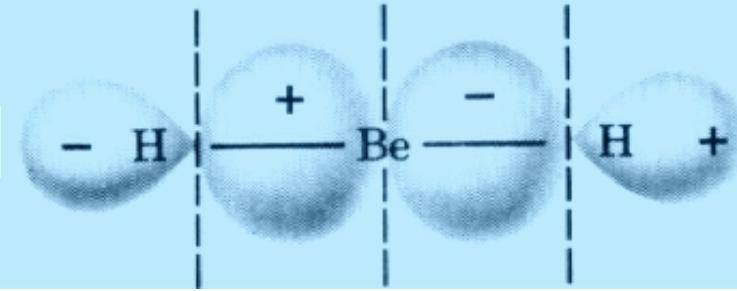
Víceatomové molekuly – BeH₂



orbitaly Be

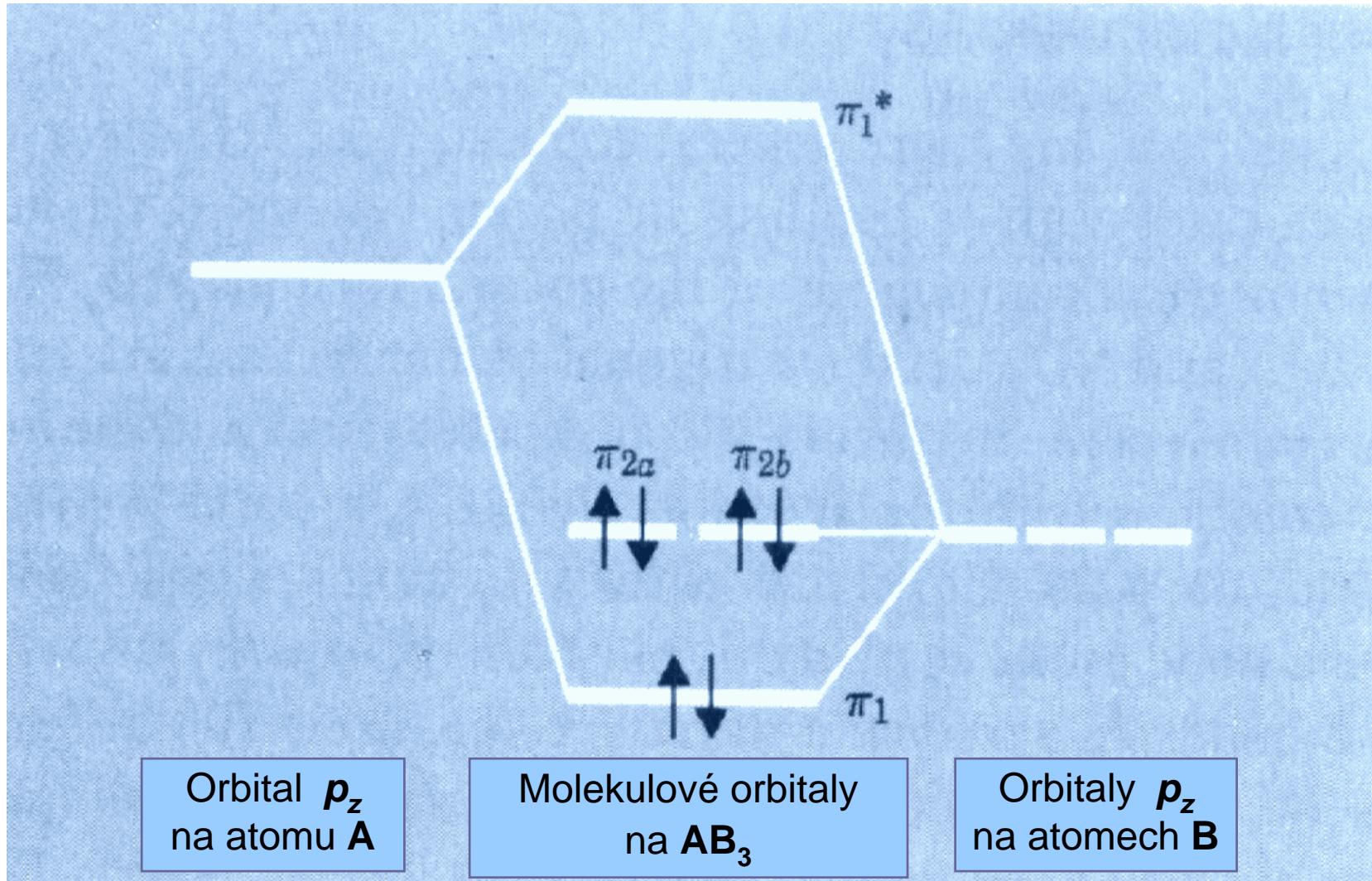
Molekulové orbitaly

orbitaly H

σ_1  σ_3  σ_2  σ_4 

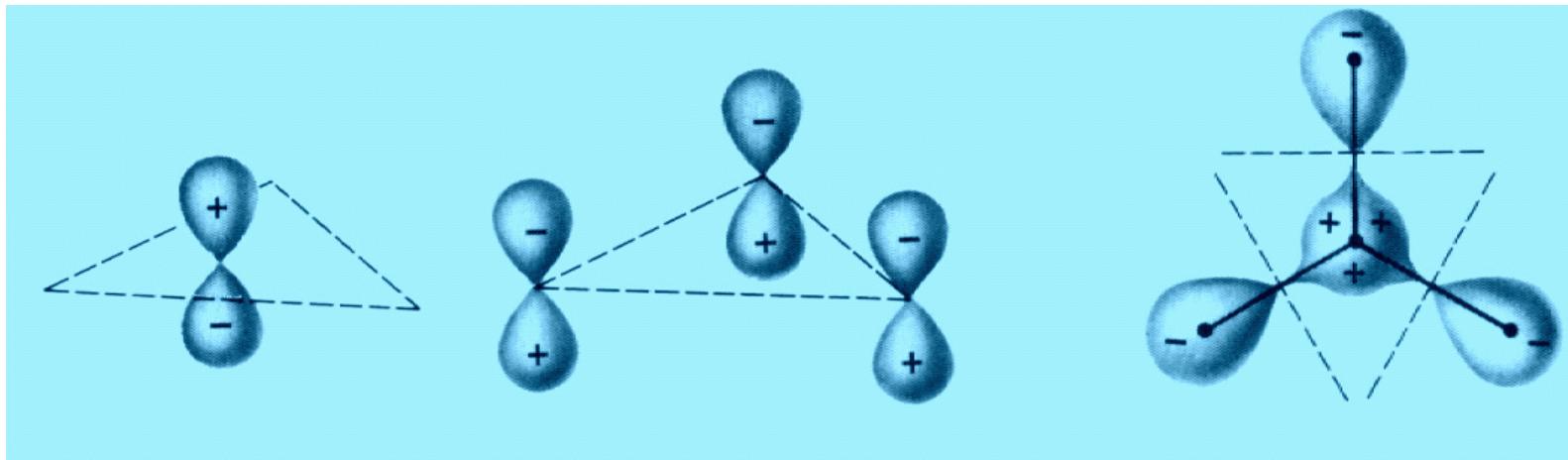
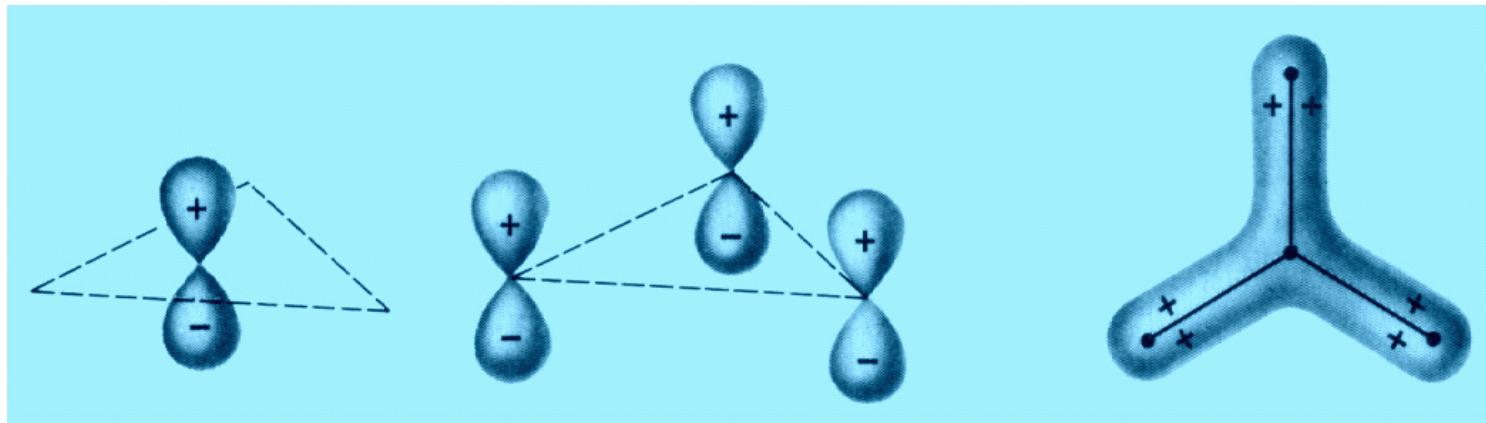
Víceatomové molekuly – BX_3

(CO_3^{2-} , NO_3^-)



Víceatomové molekuly – BX_3

(CO_3^{2-} , NO_3^-)

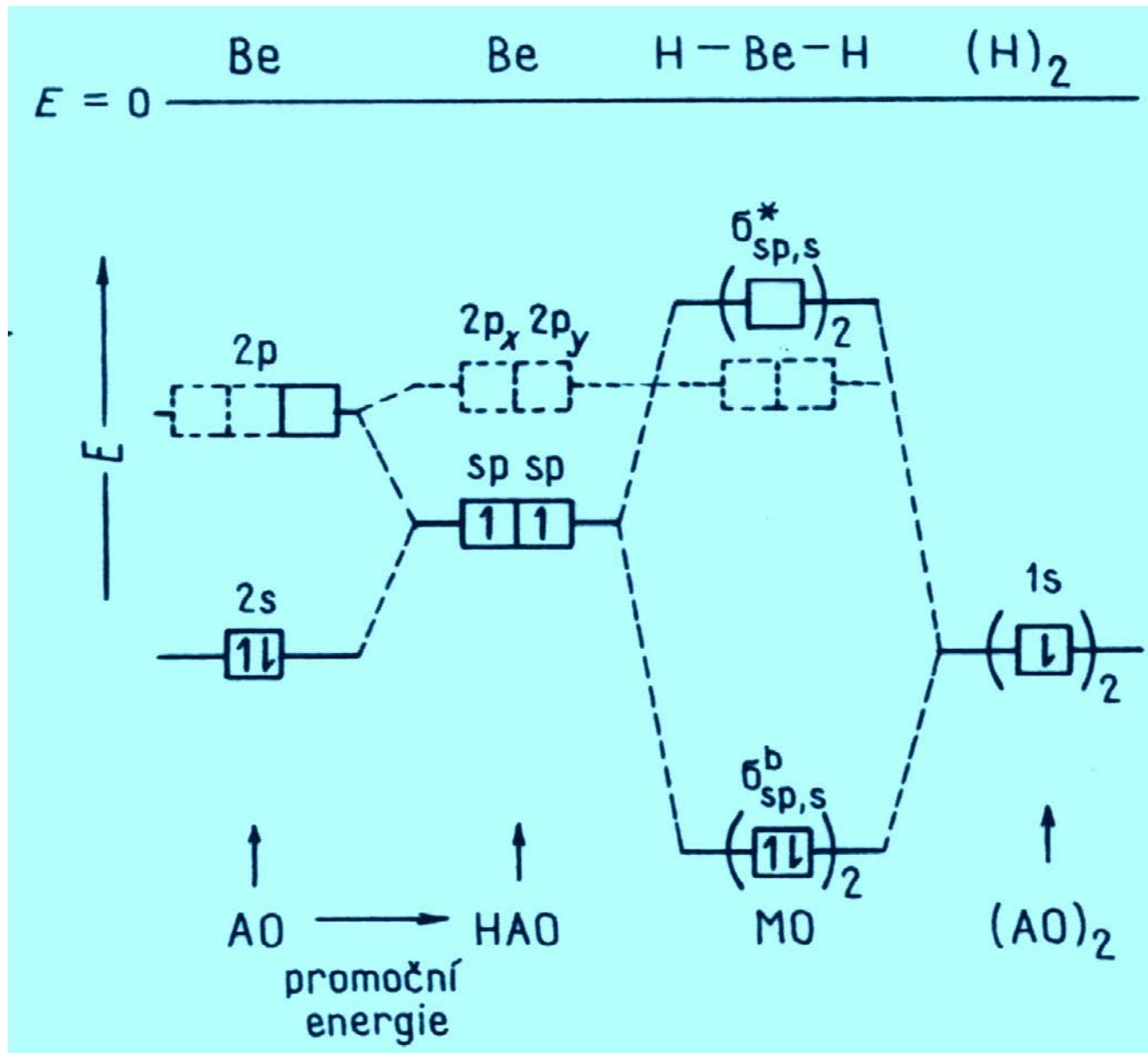


Hybridizace

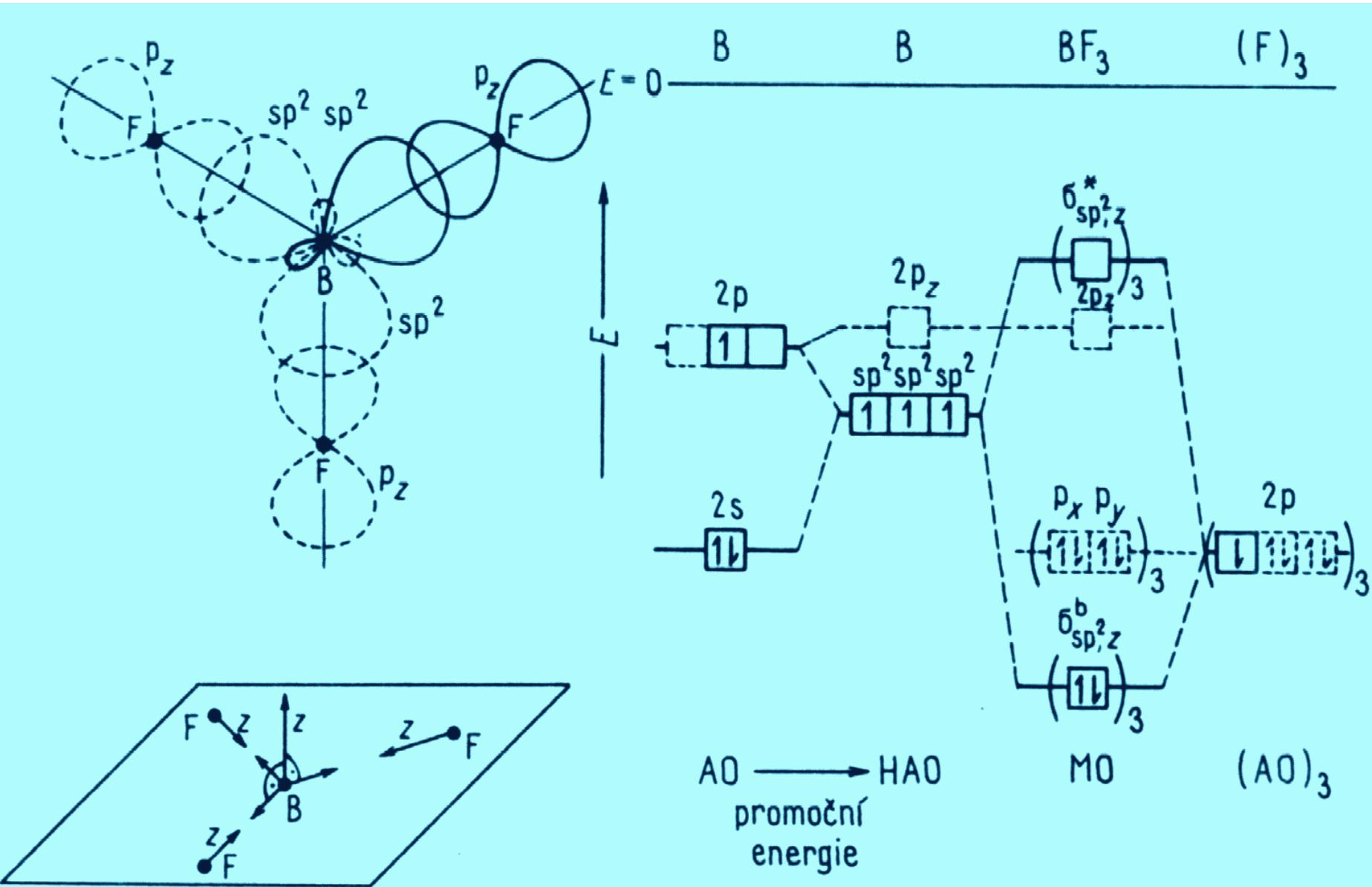
- **Energetické sjednocení atomových orbitalů**
- **V podstatě stejné jako metoda MO-LCAO**
- **V případě hybridizace jsou lineárně kombinovány orbitaly na tomtéž atomu**

Hybridizace sp

BeH₂

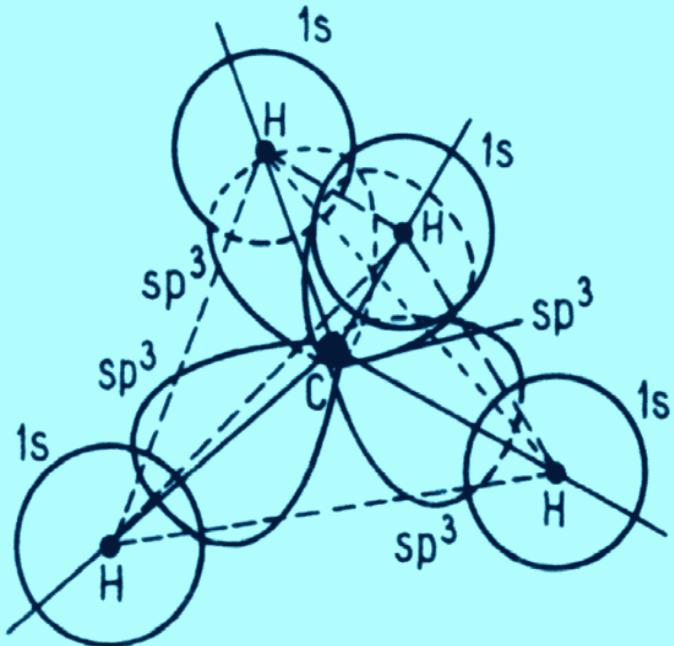


Hybridizace sp^2

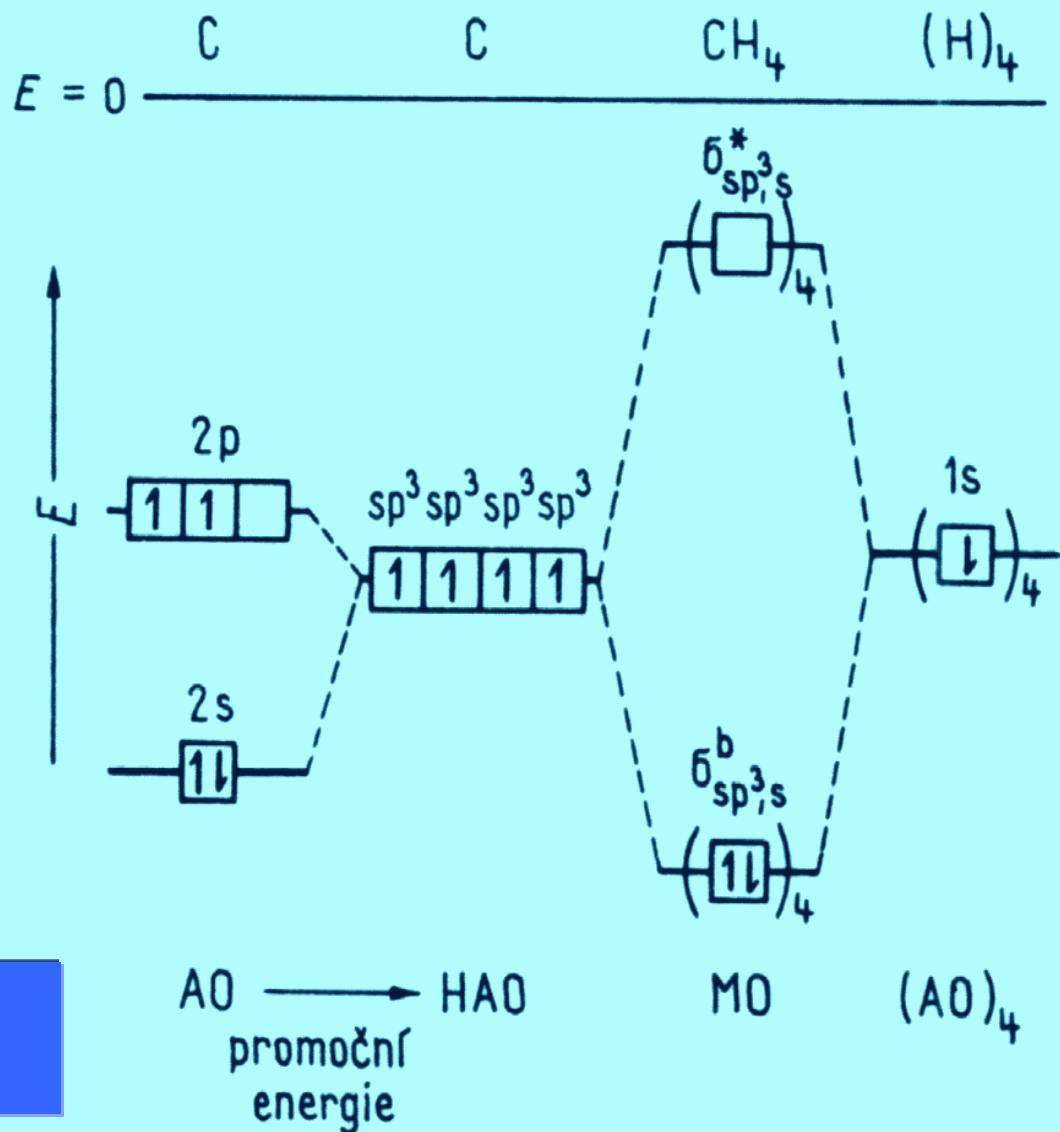


Hybridizace sp^3

CH_4

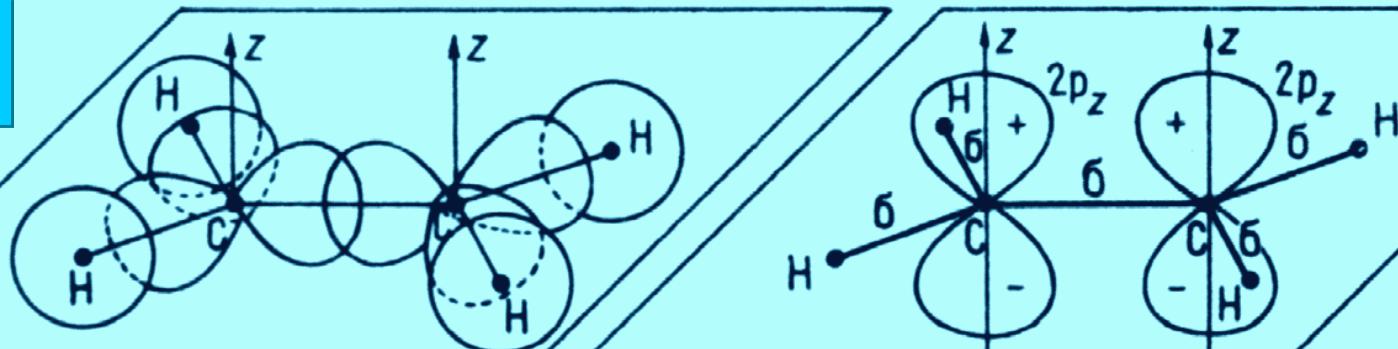


- $s, p_x, p_y, p_z \rightarrow sp^3$



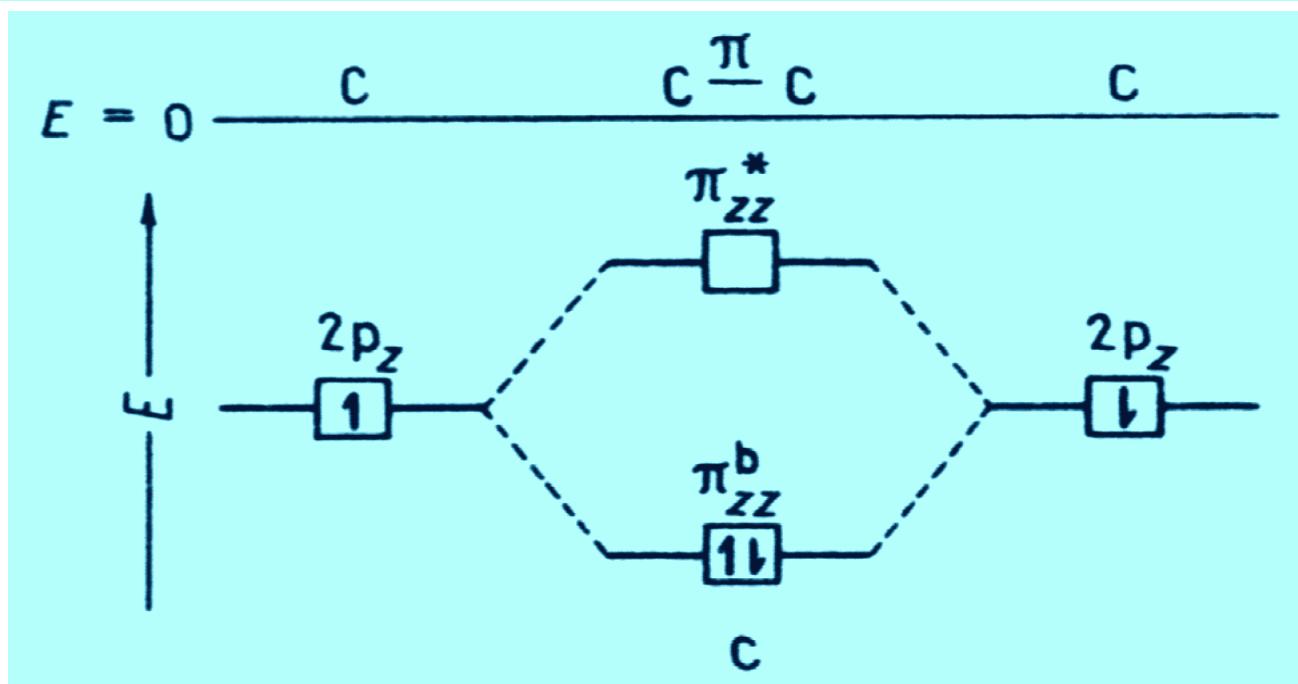
Hybridizace sp^2

C_2H_4

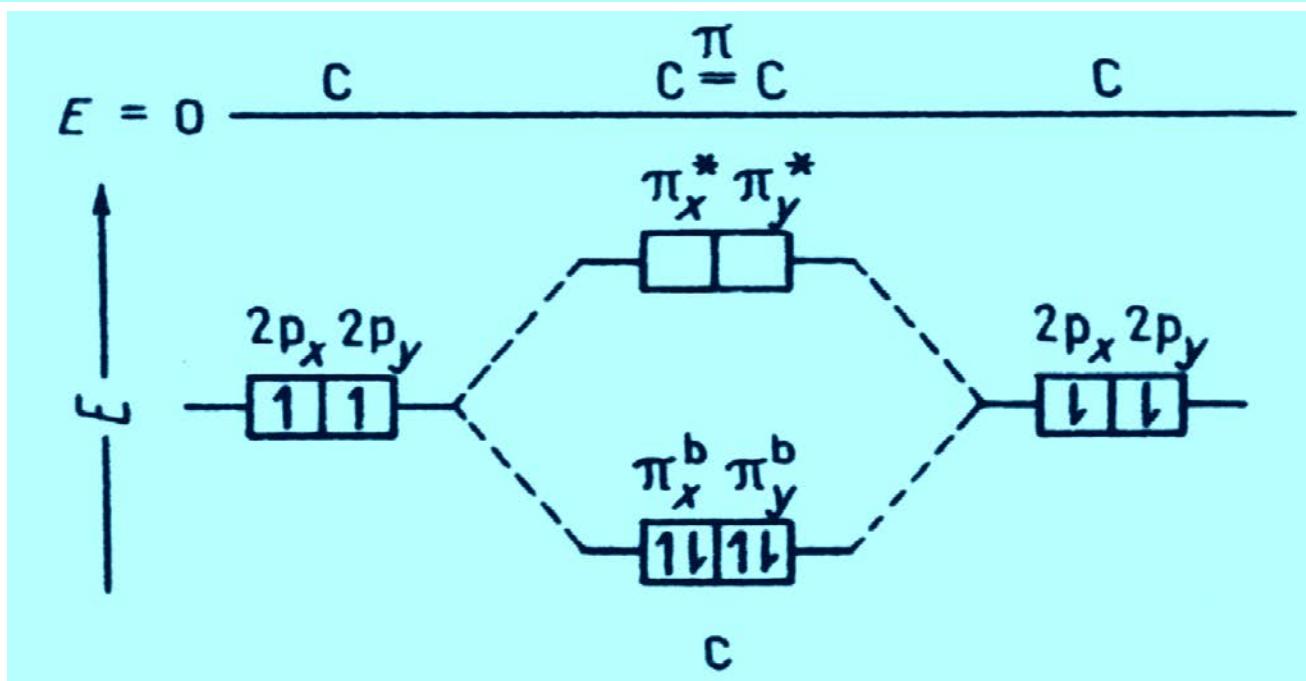
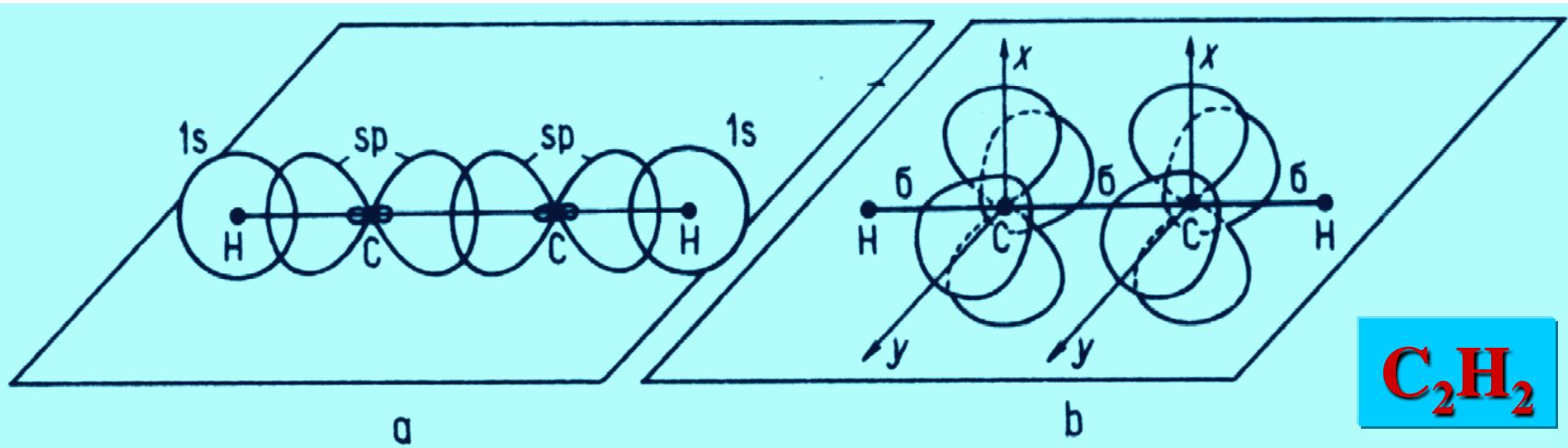


a

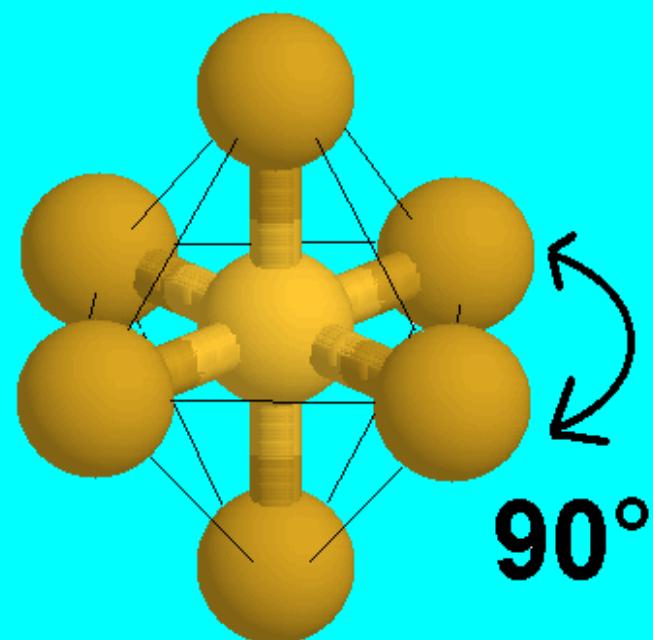
b



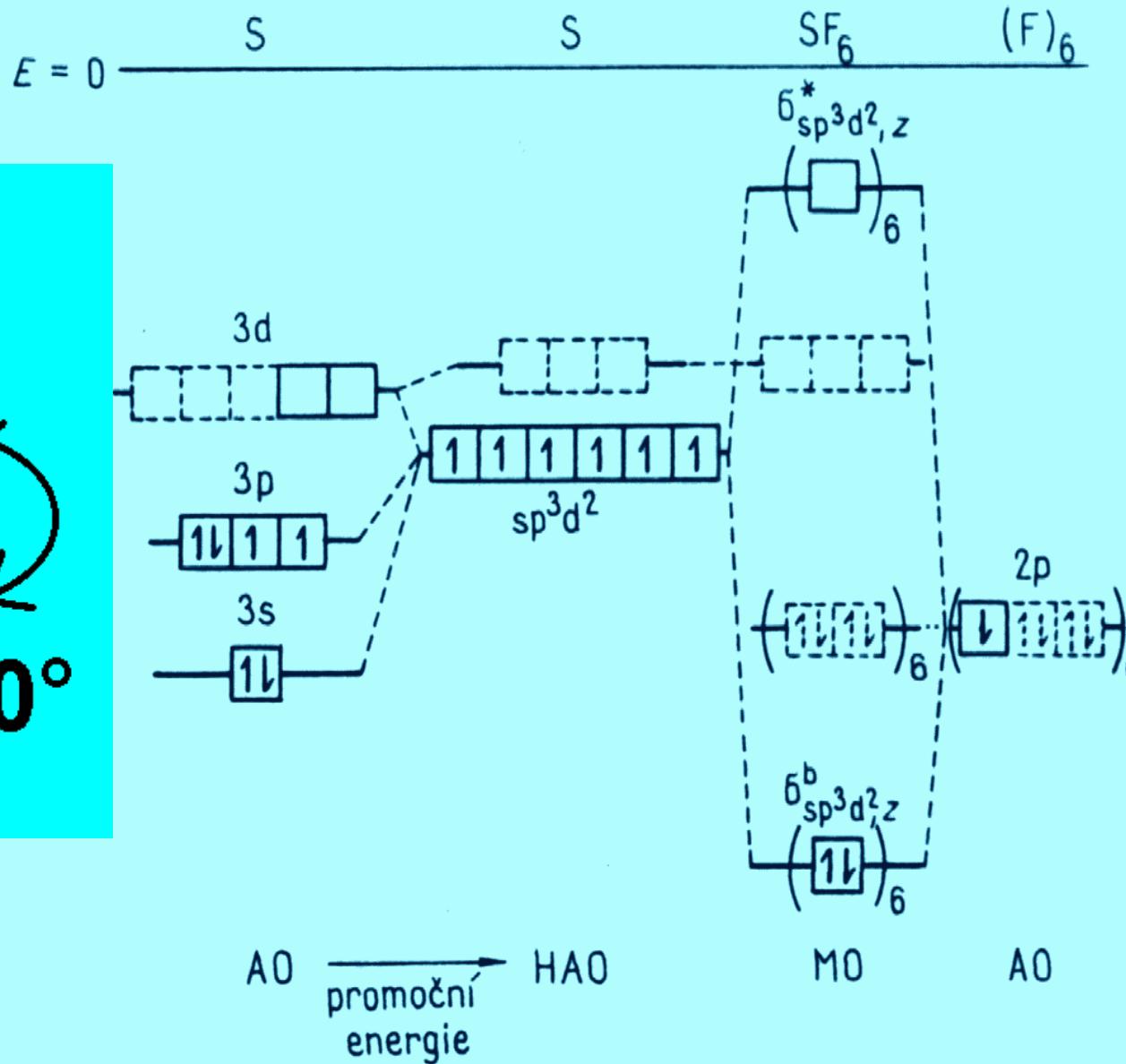
Hybridizace sp



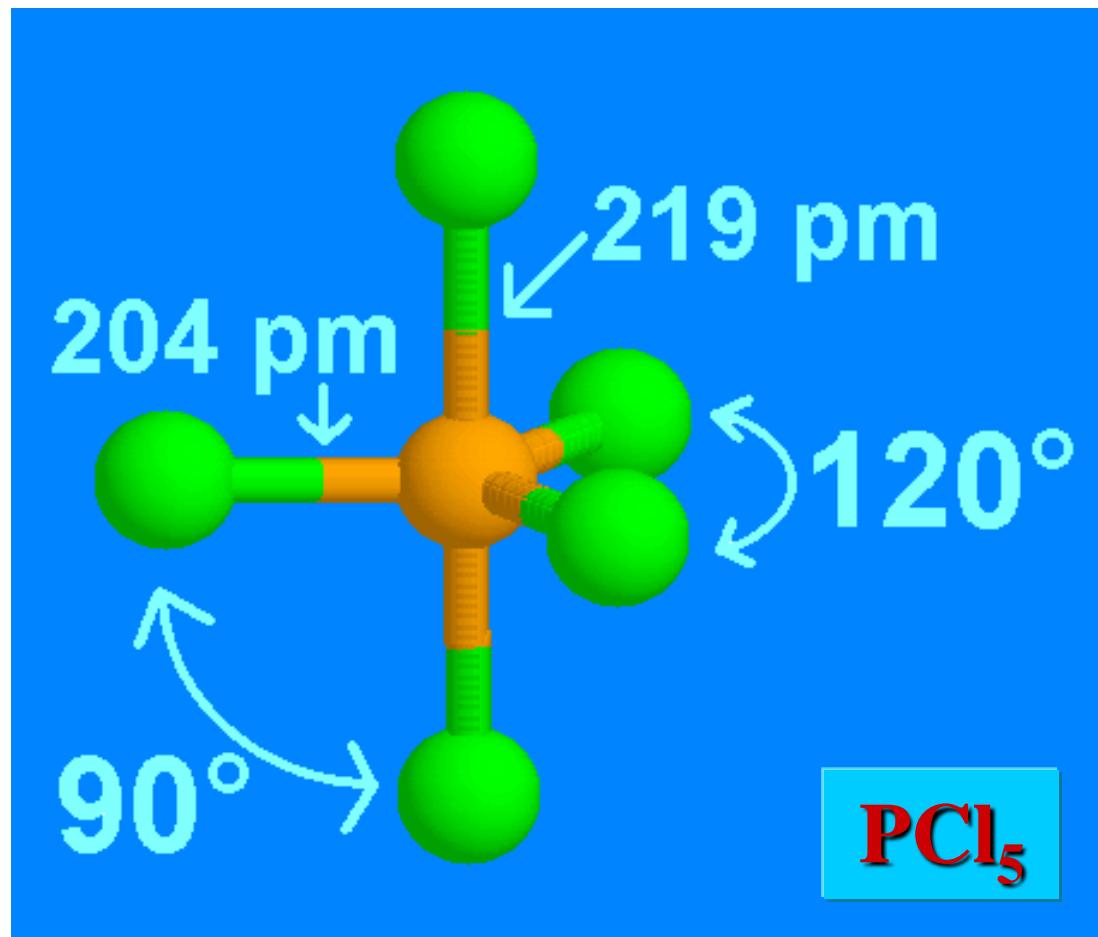
Hybridizace sp^3d^2



SF_6

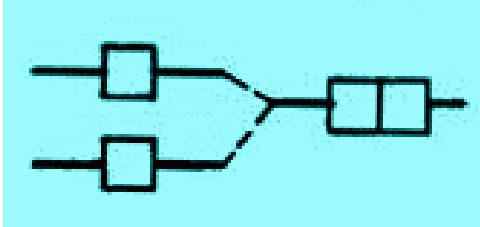
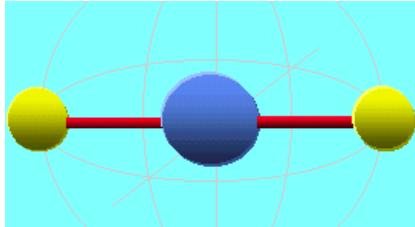
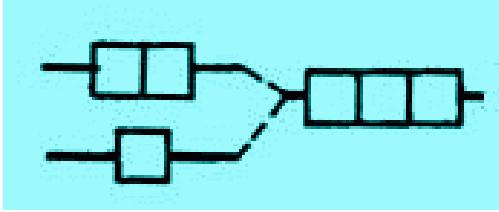
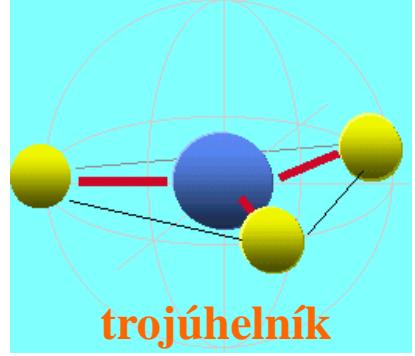
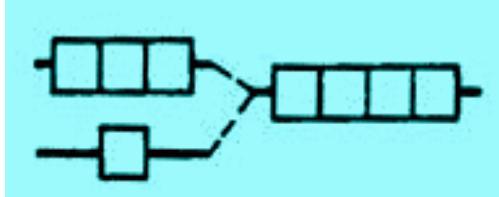
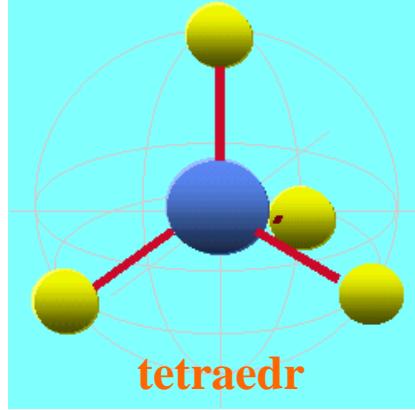


Hybridizace sp^3d

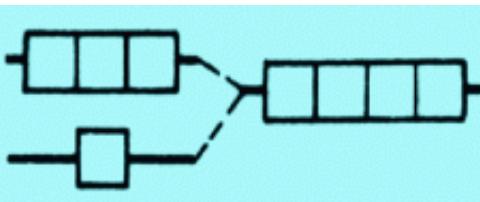
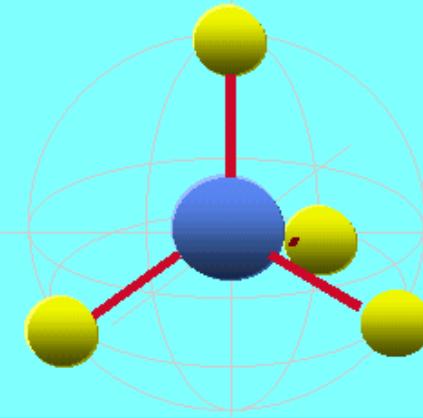
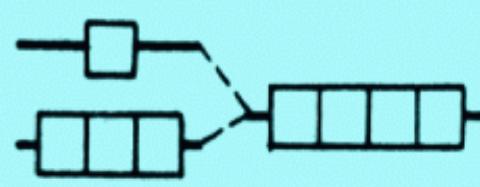
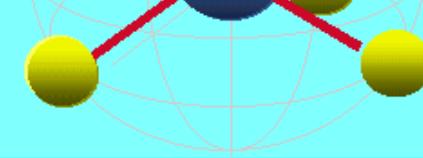
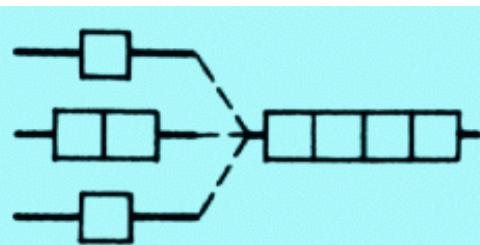
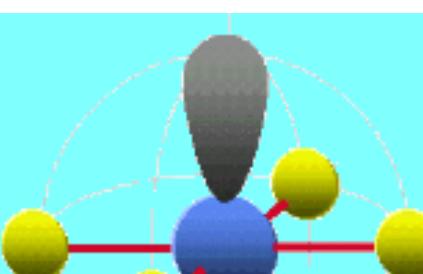
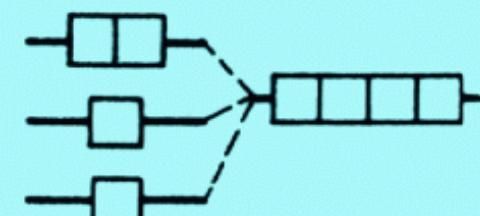


- $sp^3d = sp^2 + dp$

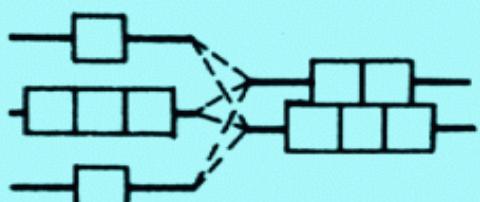
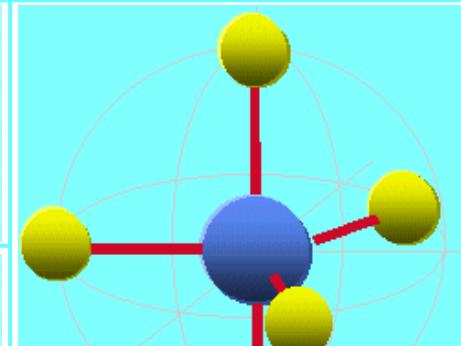
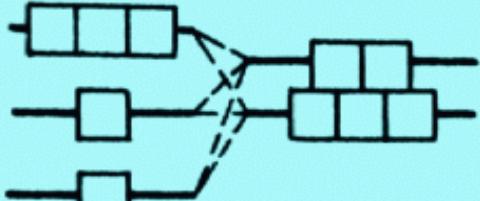
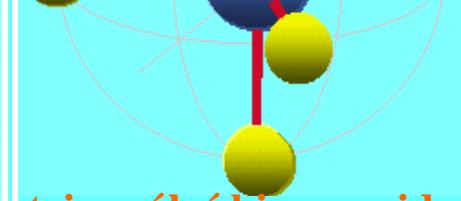
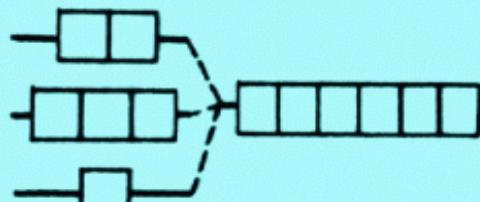
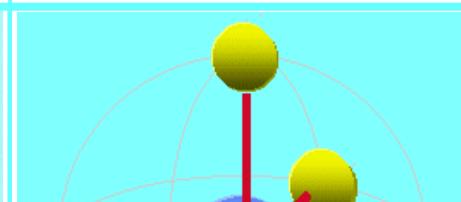
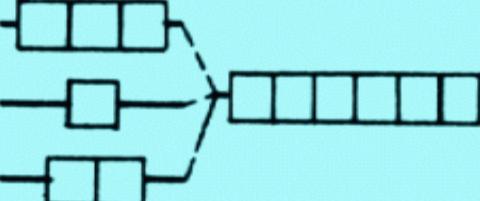
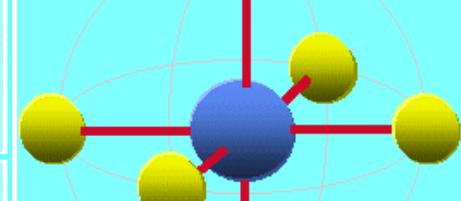
Přehled hybridizací I

typ	použité AO	energetické schéma	tvar molekuly	příklady
sp (2)	$n p_z$ $n s$			
sp² (3)	$n (p_x, p_y)$ $n s$		 trojúhelník	
sp³ (4)	$n (p_x, p_y, p_z)$ $n s$		 tetraedr	

Přehled hybridizací II

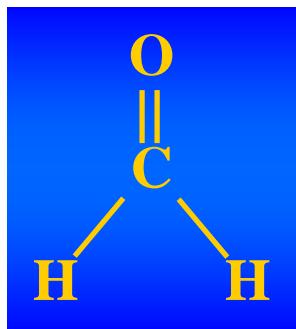
typ	použité AO	energetické schéma	tvar molekuly	příklady
sd³ (4)	$n (d_{xy}, d_{xz}, d_{yz})$ $n s$		 tetraedr (čtyřstěn)	
d³s (4)	$n s$ $(n-1) (d_{xy}, d_{xz}, d_{yz})$		 tetraedr (čtyřstěn)	
sp²d (4)	$n d_{x^2-y^2}$ $n (p_x, p_y)$ $n s$		 čtverec (planární)	
dsp² (4)	$n (p_x, p_y)$ $n s$ $(n-1) d_{x^2-y^2}$		 čtverec (planární)	

Přehled hybridizací III

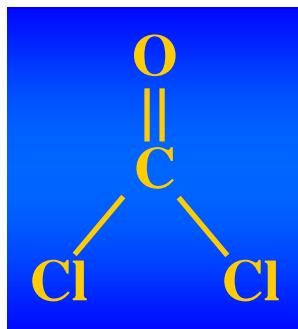
typ	použité AO	energetické schéma	tvar molekuly	příklady
$\text{sp}^3\text{d}_{z^2}$ (5)	$n \text{ d}_{z^2}$ $n (\text{p}_x, \text{p}_y, \text{p}_z)$ $n \text{ s}$			
$\text{d}_{z^2}\text{sp}^3$ (5)	$n (\text{p}_x, \text{p}_y, \text{p}_z)$ $n \text{ s}$ $(n-1) \text{ d}_{z^2}$		 trigonální bipyramida	
$\text{sp}^3\text{d}^{(2)}$ (5/6)	$n \text{ d}_{x^2-y^2}$ $n (\text{p}_x, \text{p}_y, \text{p}_z)$ $n \text{ s}$			
$\text{d}^{(2)}\text{sp}^3$ (6/5)	$n (\text{p}_x, \text{p}_y, \text{p}_z)$ $n \text{ s}$ $(n-1) \text{ d}_{x^2-y^2}$		 oktaedr (osmistěn)	

Ovlivnění hybridních orbitalů a tvaru molekuly

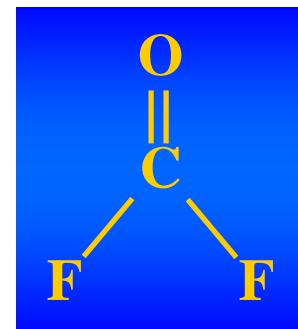
1) Vliv π orbitalů



$$\angle \text{HCH} = 116^\circ$$



$$\angle \text{ClCCl} = 111^\circ$$

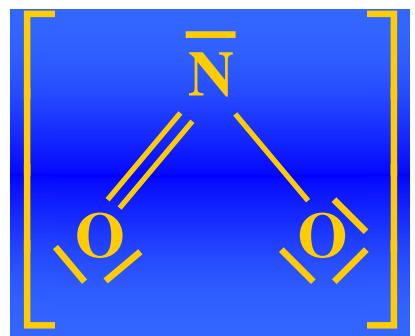


$$\angle \text{FCF} = 108^\circ$$

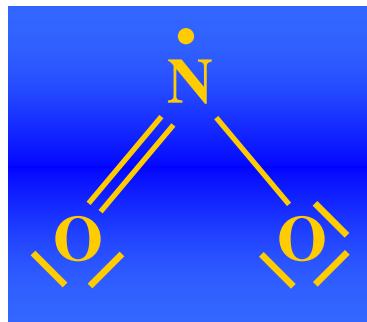
Ovlivnění hybridních orbitalů a tvaru molekuly

1) Vliv π orbitalů

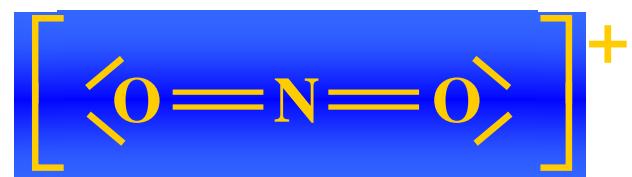
2) Vliv volných elektronových párů



$$\angle \text{ONO} = 115^\circ$$



$$\angle \text{ONO} = 132^\circ$$



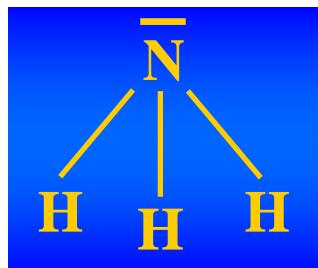
$$\angle \text{ONO} = 180^\circ$$

Ovlivnění hybridních orbitalů a tvaru molekuly

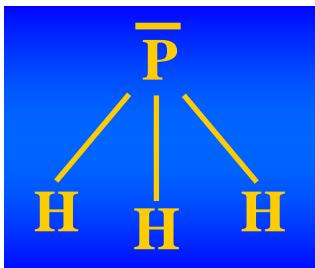
1) Vliv π orbitalů

2) Vliv volných elektronových párů

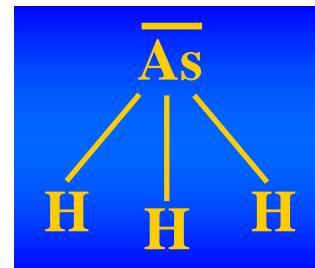
3) Odhybridizování



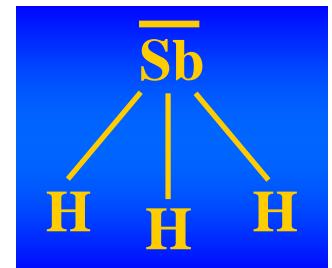
$$\angle \text{HNH} = 107^\circ$$



$$\angle \text{HPH} = 94^\circ$$



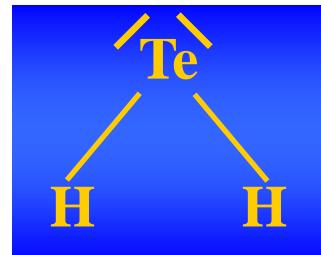
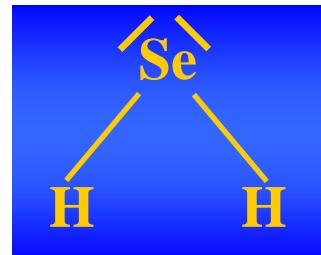
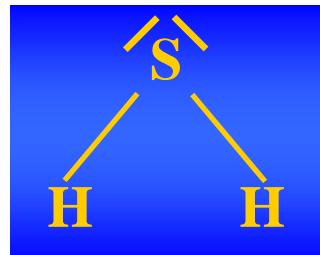
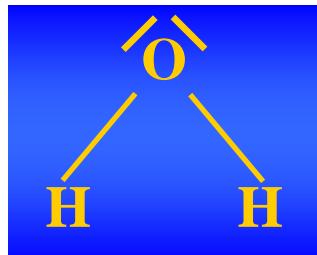
$$\angle \text{HAsH} = 92^\circ$$



$$\angle \text{HSbH} = 91^\circ$$

Ovlivnění hybridních orbitalů a tvaru molekuly

- 1) Vliv π orbitalů
- 2) Vliv volných elektronových párů
- 3) Odhybridizování



$$\angle \text{HOH} = 104^\circ$$

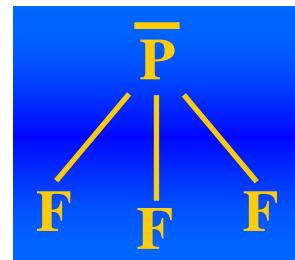
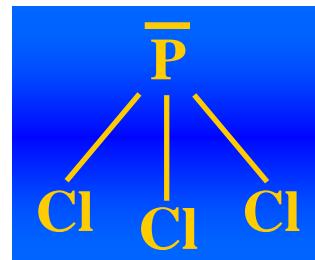
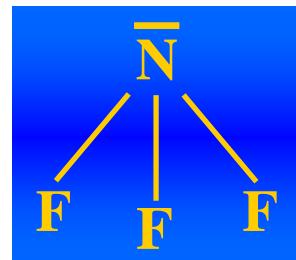
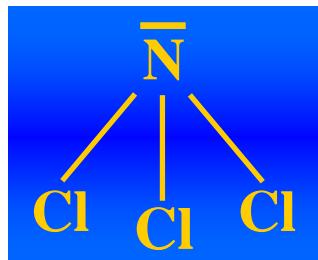
$$\angle \text{HSH} = 92^\circ$$

$$\angle \text{HSeH} = 91^\circ$$

$$\angle \text{HTeH} = 90^\circ$$

Ovlivnění hybridních orbitalů a tvaru molekuly

- 1) Vliv π orbitalů
- 2) Vliv volných elektronových párů
- 3) Odhybridizování
- 4) Velikost atomů



$$\angle \text{CINCl} = 107^\circ$$

$$\angle \text{FNF} = 102^\circ$$

$$\angle \text{CIPCl} = 100^\circ$$

$$\angle \text{FPF} = 98^\circ$$

VSEPR

= Valence-shell electron-pair repulsion

geometrie molekuly – minimum celkové energie v prostoru souřadnic všech atomů

- | | |
|-------------------------|---------------------------------------|
| energie molekuly | → repulze mezi elektrony |
| | → repulze mezi jádry |
| | → přitažlivá energie mezi el. a jádry |
| | → kinetická energie elektronů |

- uvažuje pouze repulzi valenčních elektronových párů
- jejich prostorové uspořádání odpovídá minimu odpudivé energie

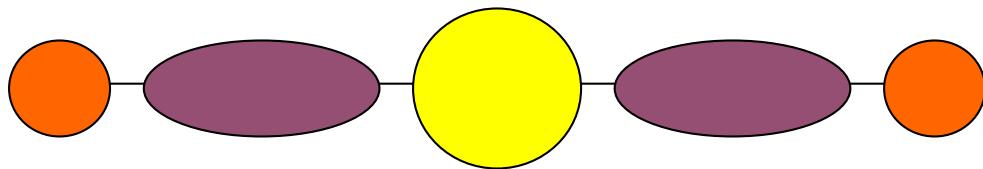
VSEPR

- Elektronový pár se snaží co nejvíce přiblížit k jádru a zároveň být co nejdále od ostatních elektronových párů
- Repulze mezi elektronovými páry klesá v pořadí:
 - 2 nevazebné (volné) elektronové páry**
 - vazebný pár – nevazebný pár
 - 2 vazebné elektronové páry**
- Mezi strukturami s 90° interakcemi je upřednostněna konfigurace s minimem těchto interakcí

VSEPR – 2 elektronové páry

základní tvar – lineární

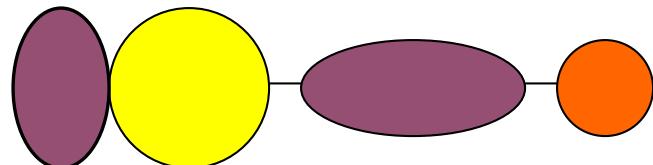
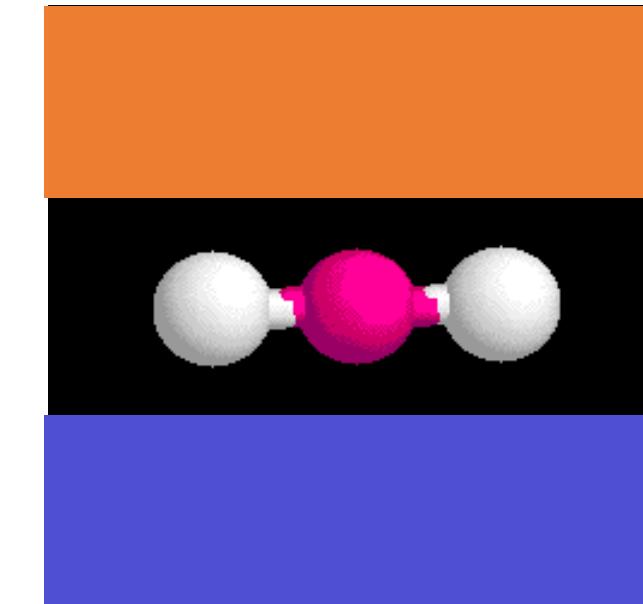
AB₂ – 0 volných el. párů



Příklady: BeCl₂, CO₂, HgCl₂, ZnI₂, CdBr₂, N³⁻

AXE – 1 volný el. pár

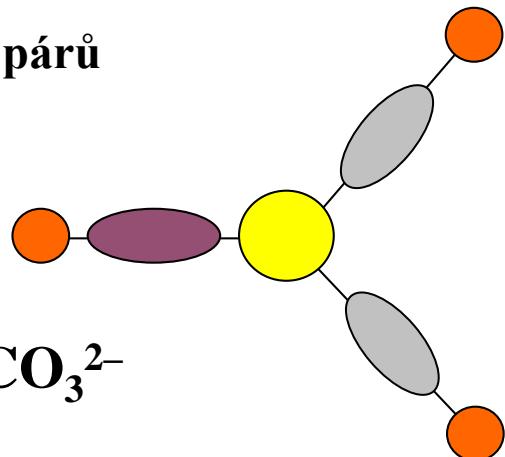
odvozený tvar – lineární



VSEPR – 3 elektronové páry

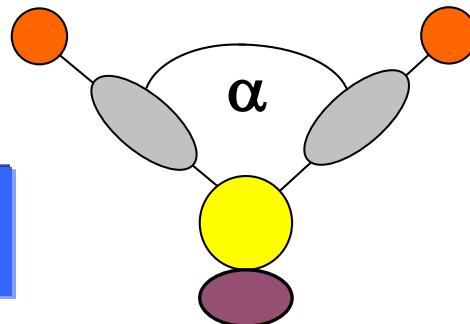
**základní tvar –
rovnoramenný trojúhelník**

AB₃ – 1 volných el. párů

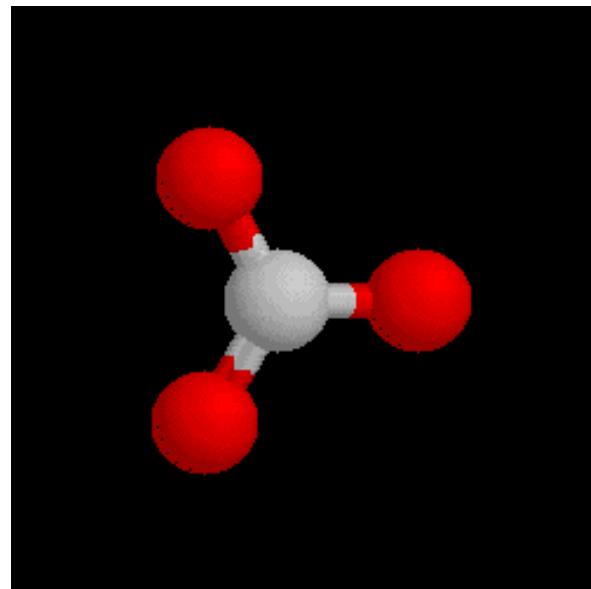


Příklady: BCl₃, NO₃⁻, CO₃²⁻

AX₂E – 1 volný el. pár



odvozený tvar – lomený



Příklady:
O₃, SO₂, NO₂⁻, SnCl₂

VSEPR – 4 elektronové páry

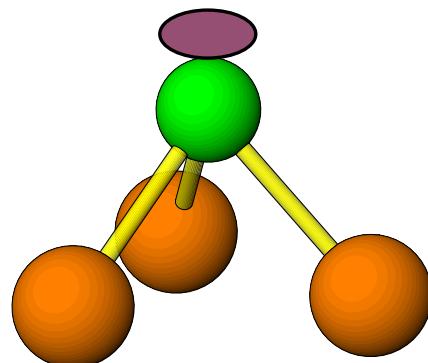
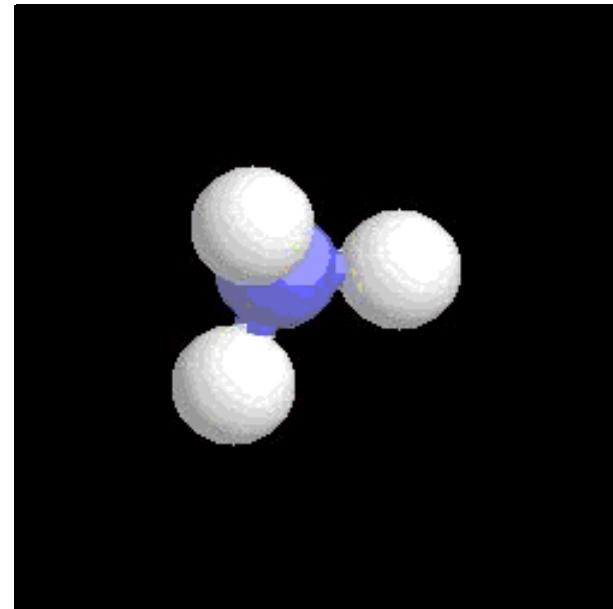
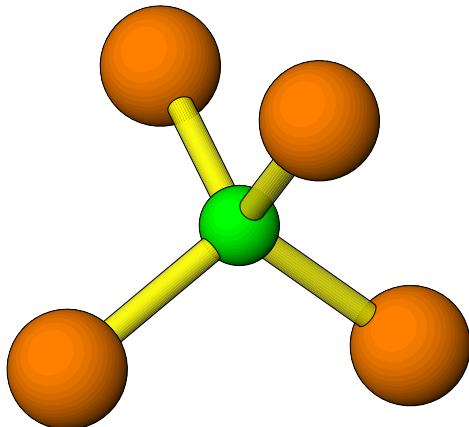
**základní tvar –
tetraedr (čtyřstěn)**

AB₄ – 0 volných el. párů

Příklady: CH₄, ClO₄⁻,
SO₄²⁻, NH₄⁺

AX₃E – 1 volný el. pár

**odvozený tvar –
trigonální pyramida**



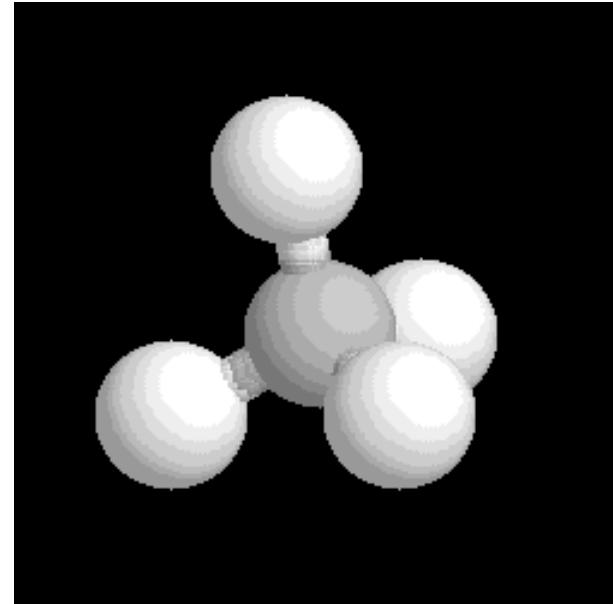
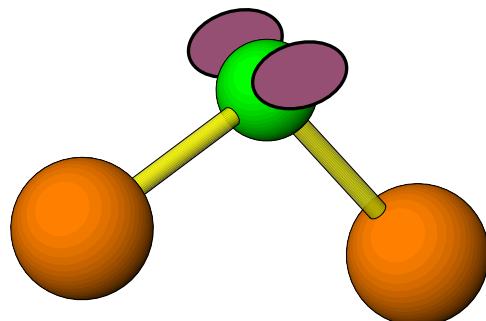
Příklady:
NH₃, PF₃, SO₃²⁻,
H₃O⁺, ClO₃⁻

VSEPR – 4 elektronové páry

AX₂E₂ – 2 volné el. páry

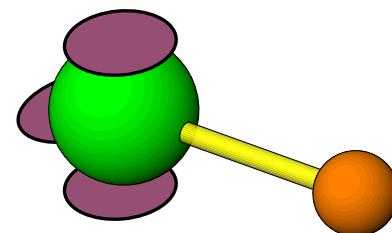
odvozený tvar – lomený

Příklady: H₂O, H₂S,
SCl₂, ClO₂⁻



AXE₃ – 3 volné el. páry

odvozený tvar – lineární



Příklady:
HCl, OH⁻

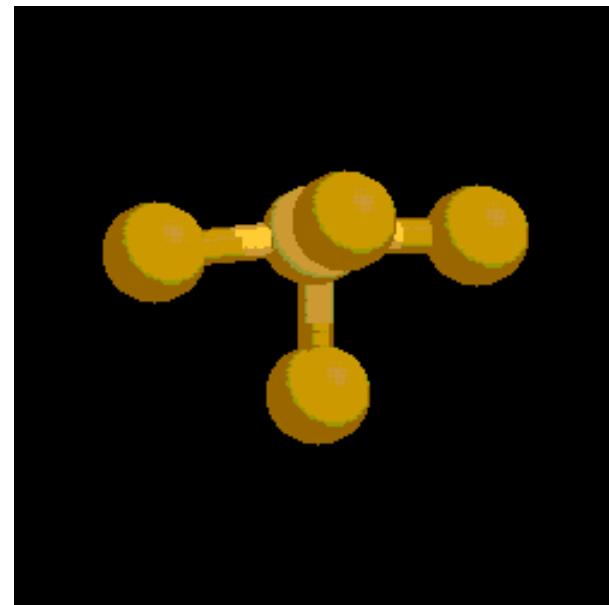
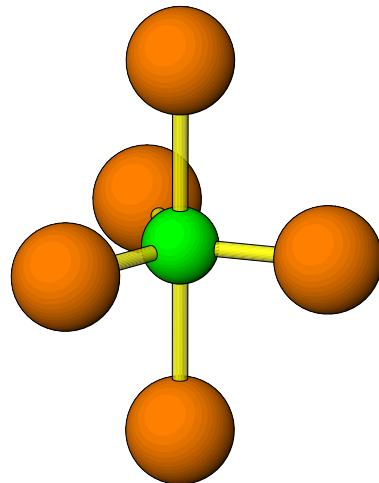
VSEPR – 5 elektronových párů

**základní tvar –
trigonální bipyramida**

AB₅ – 1 volných el. párů

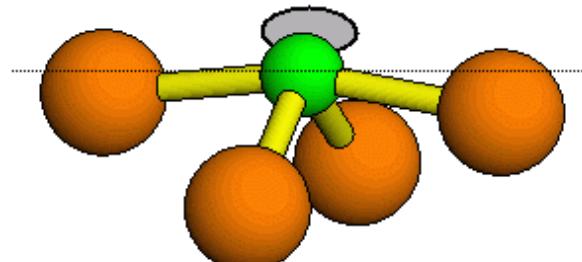
Příklady:

PCl₅, AsF₅, PF₃(CH₃)₂



AX₄E – 1 volný el. pár

**odvozený tvar –
„seesaw“ (houpačka),
deformovaný tetraedr**

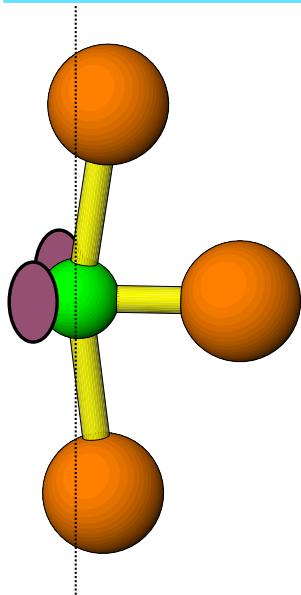


Příklady:
SF₄, R₂TeCl₂

VSEPR – 5 elektronových párů

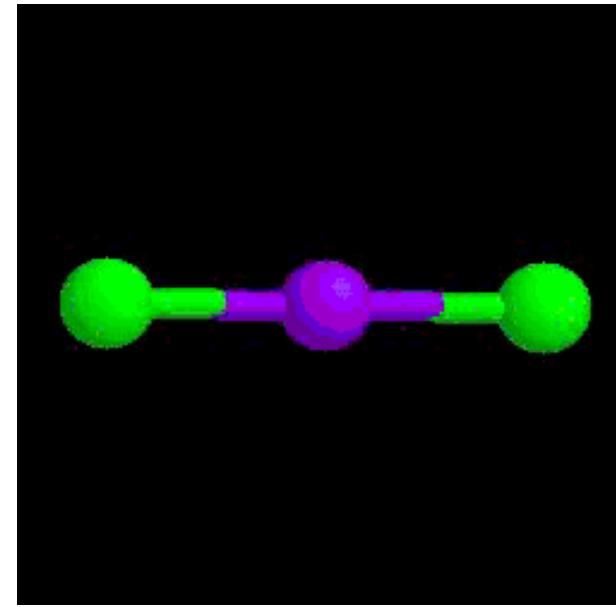
AX₃E₂

– **2** volné el. páry



odvozený tvar – tvar T

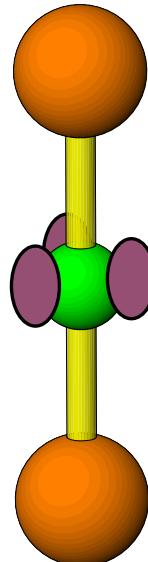
Příklady: ClF₃, BrF₃,
(C₆H₅)ICl₂



AX₂E₃

– **3** volné el. páry

odvozený tvar – lineární



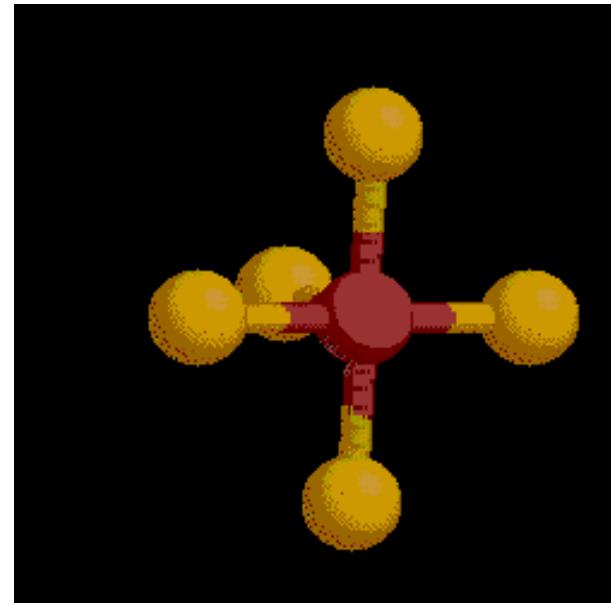
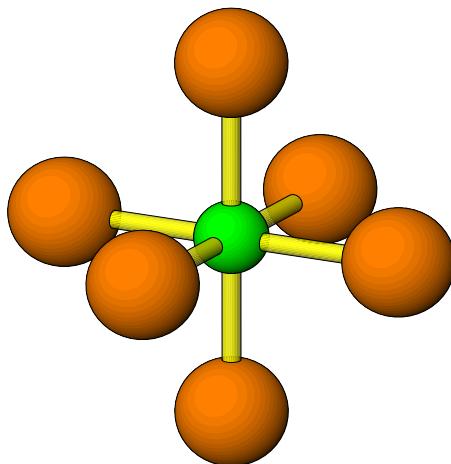
Příklady:
XeF₂, ICl₂⁻, I₃⁻

VSEPR – 6 elektronových párů

**základní tvar –
oktaedr (osmistěn)**

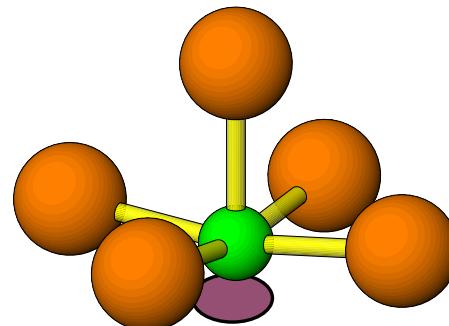
AB₆ – 0 volných el. párů

Příklady:
SF₆, SeF₆, PCl₆⁻, SiF₆²⁻



AX₅E – 1 volný el. pár

**odvozený tvar –
tetragonální pyramida**



Příklady:
ClF₅, BrF₅,
IF₅, XeOF₄

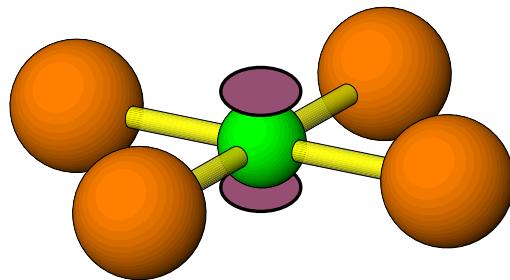
VSEPR – 6 elektronových párů

AX₄E₂ – 2 volné el. páry

odvozený tvar – čtverec

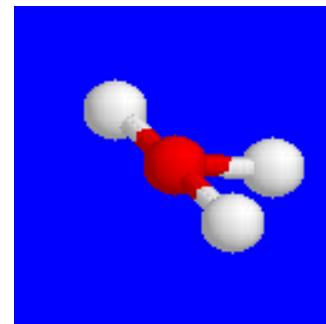
Příklady:

ClF₄, ICl₄⁻, XeF₄



AX₃E₃ – 3 volné el. páry

odvozený tvar – tvar T

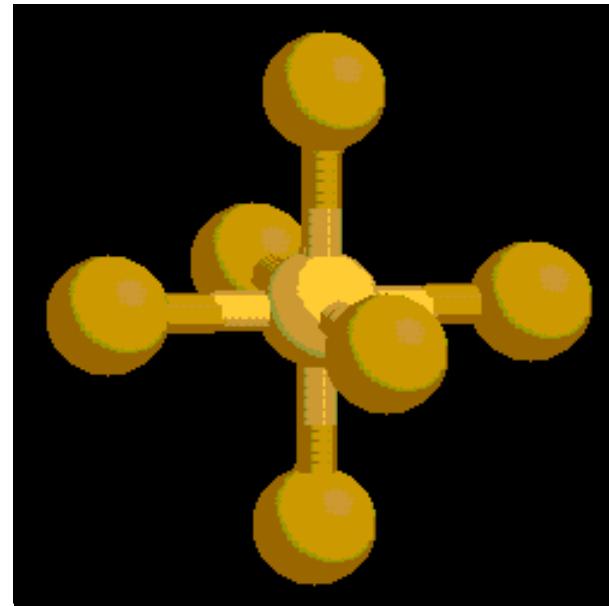


Příklad: XeF₃⁻

AX₂E₄ – 4 volné el. páry

AXE₅ – 5 volných el. párů

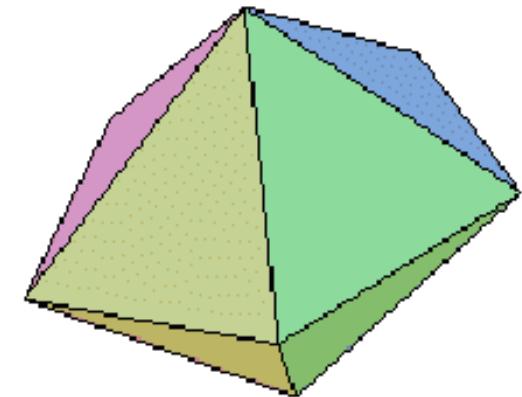
odvozený tvar – lineární



Vyšší koordinace (7 – 9)

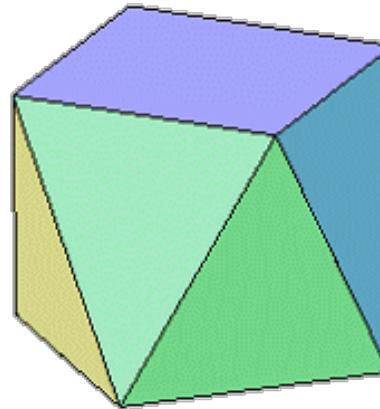
k.č. 7

- pentagonální bipyramida (Př.: IF_7)
- „capped“ oktaedr
- „capped“ trigonální prizma



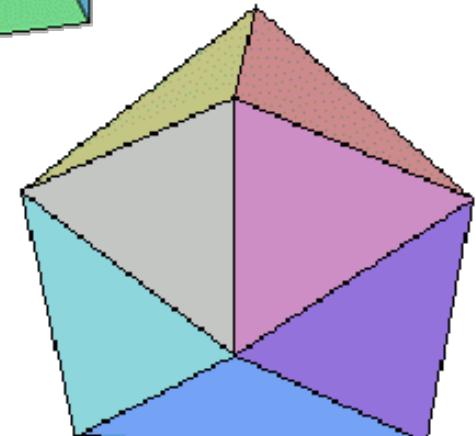
k.č. 8

- tetragonální prizma
(Př.: TaF_8^{3-})
- trigonální dodekaedr
(12-tistěn)

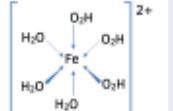
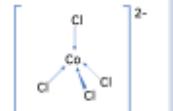
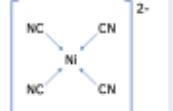
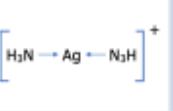
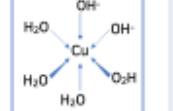


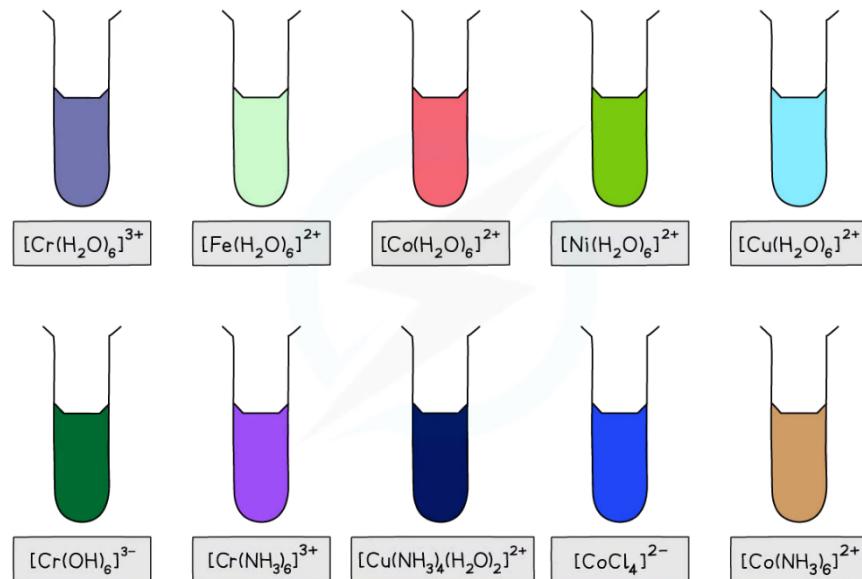
k.č. 9

- „capped“ (3×) trigonální prizma
(Př.: ReH_9^{2-})



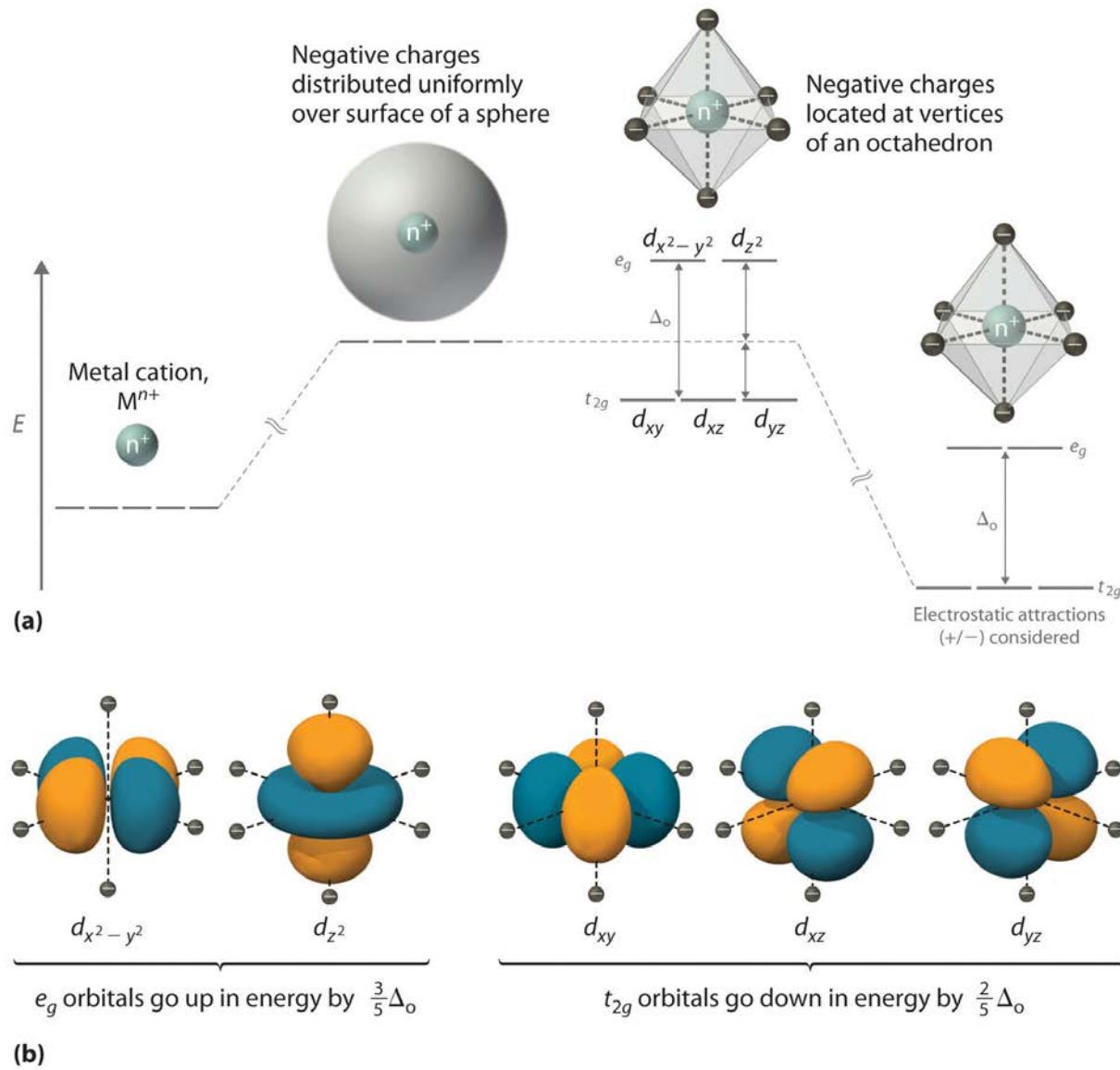
Komplexní sloučeniny

Structure	Central Atom	Ligand(s)	Ligand n°	Name
	Iron (II)	Water	6	Hexa-aquo-iron (II) ion
	Cobalt (II)	Chlorine	4	Tetra-chloro-cobalt (II) ion
	Nickel (II)	Cyanide	4	Tetra-cyano-nickel (II) ion
	Silver	Ammonia	2	Diamminesilver ion
	Copper (II)	Water Hydroxide ions	2 3	Di-hydroxy-tetra-aquo-copper (II)

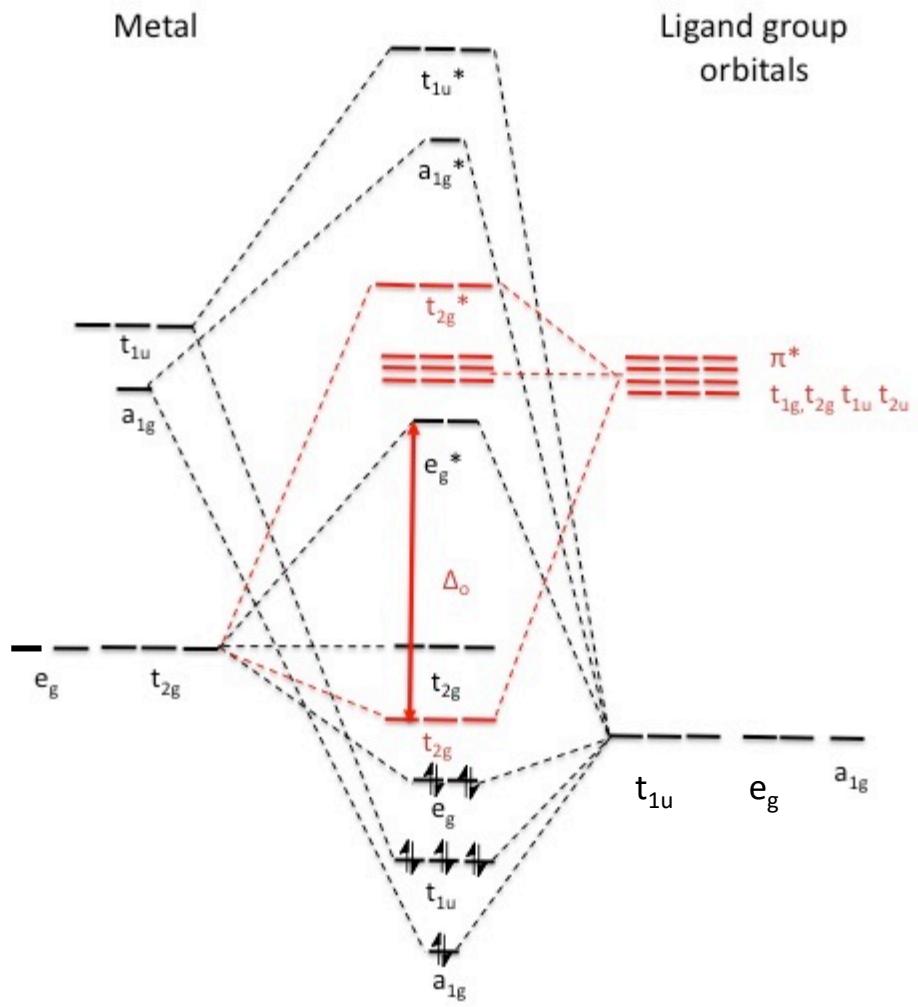
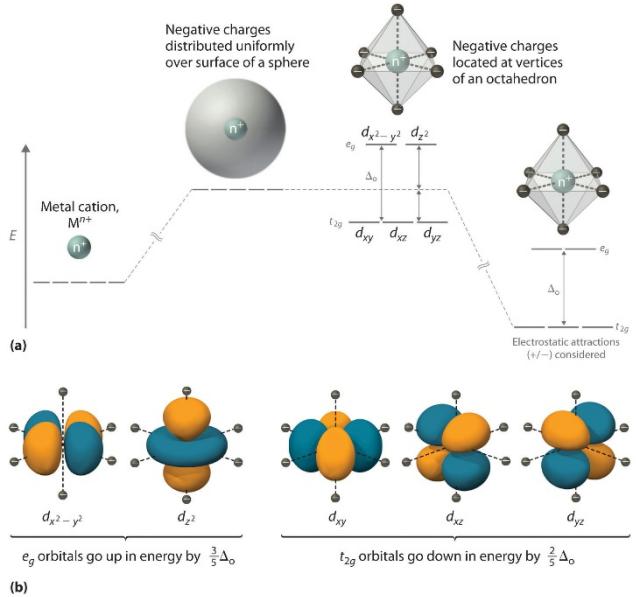


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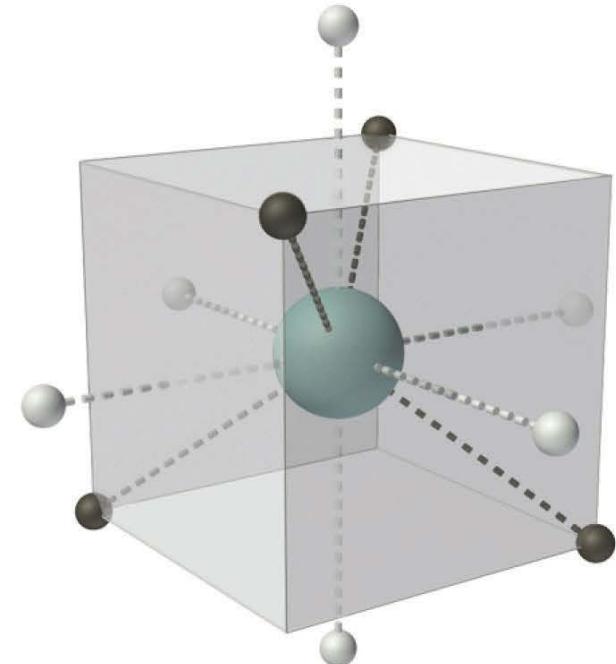
MO diagram – komplexní sloučeniny



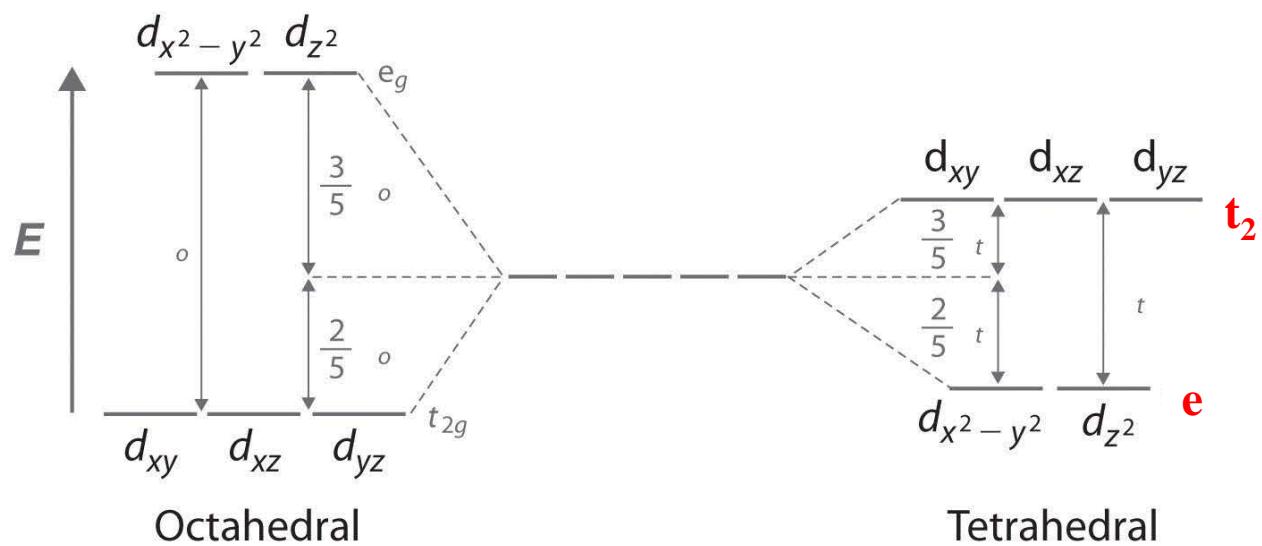
MO diagram – komplexní sloučeniny



MO diagram – komplexní sloučeniny

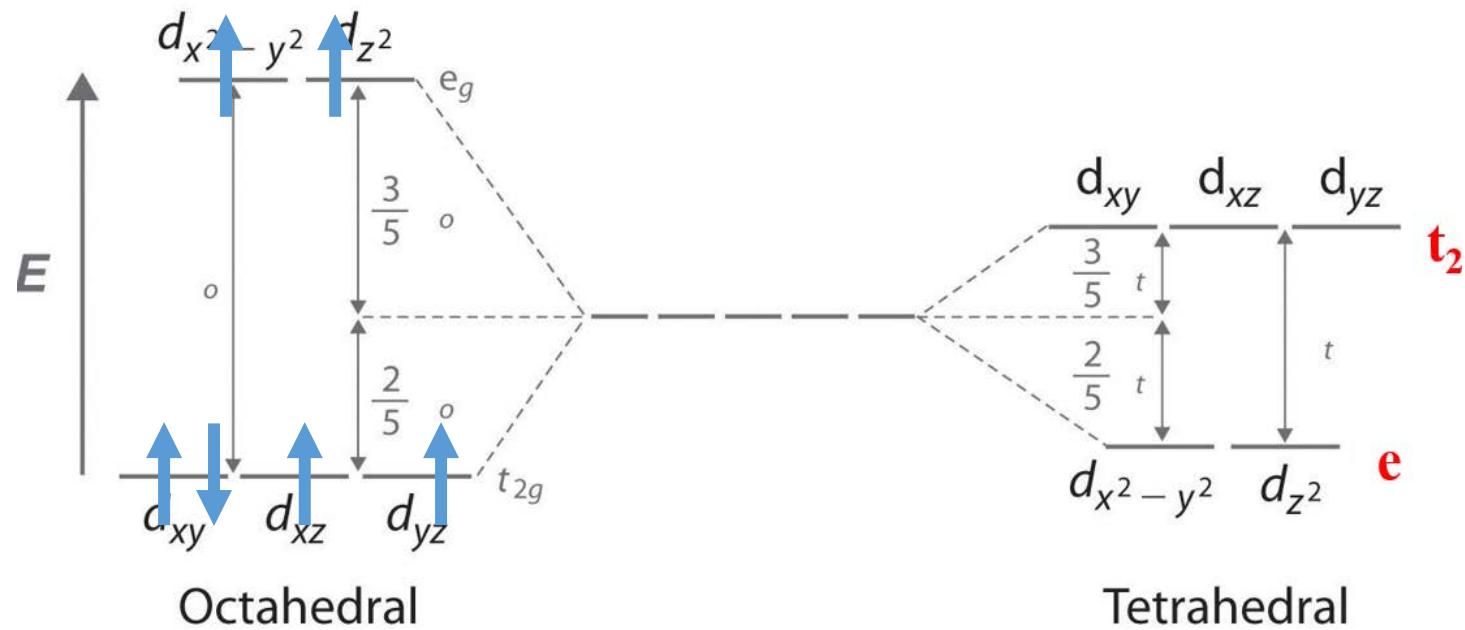


(a)



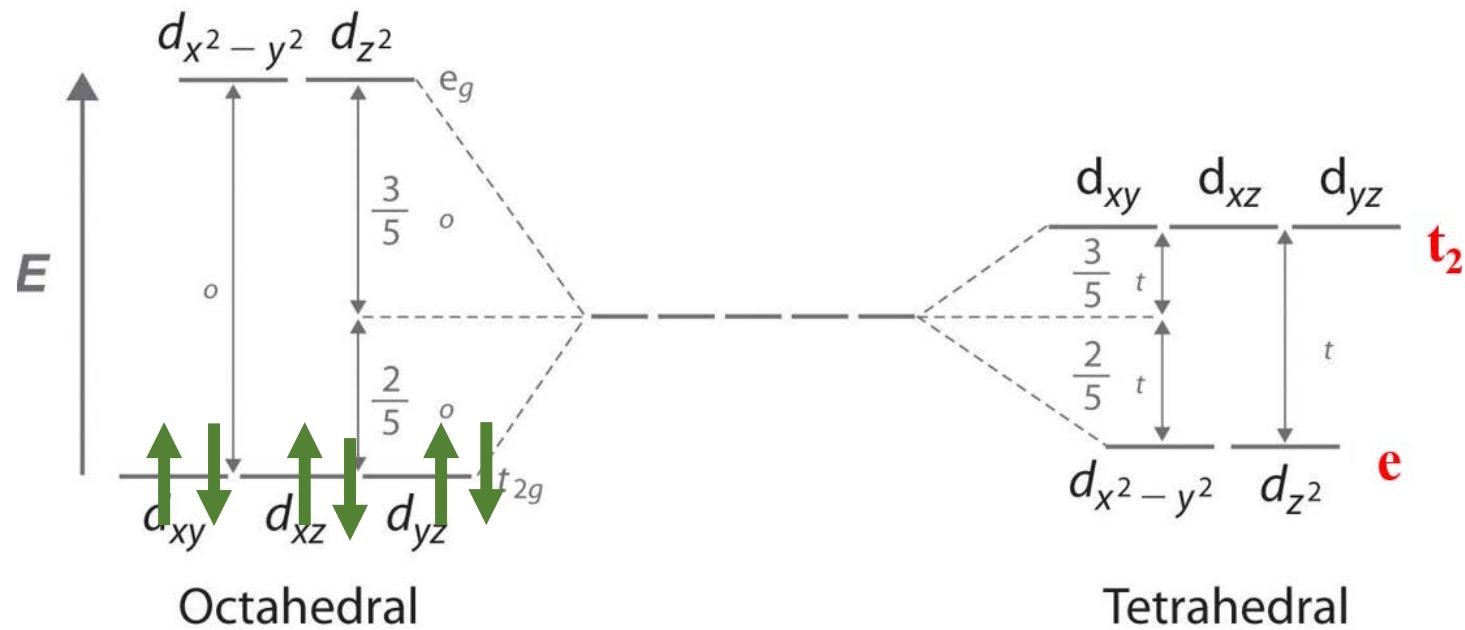
(b)

Vysoko a nízkospinové komplexy (HS, LS)



d^6 HS ... 4 nepárové el.

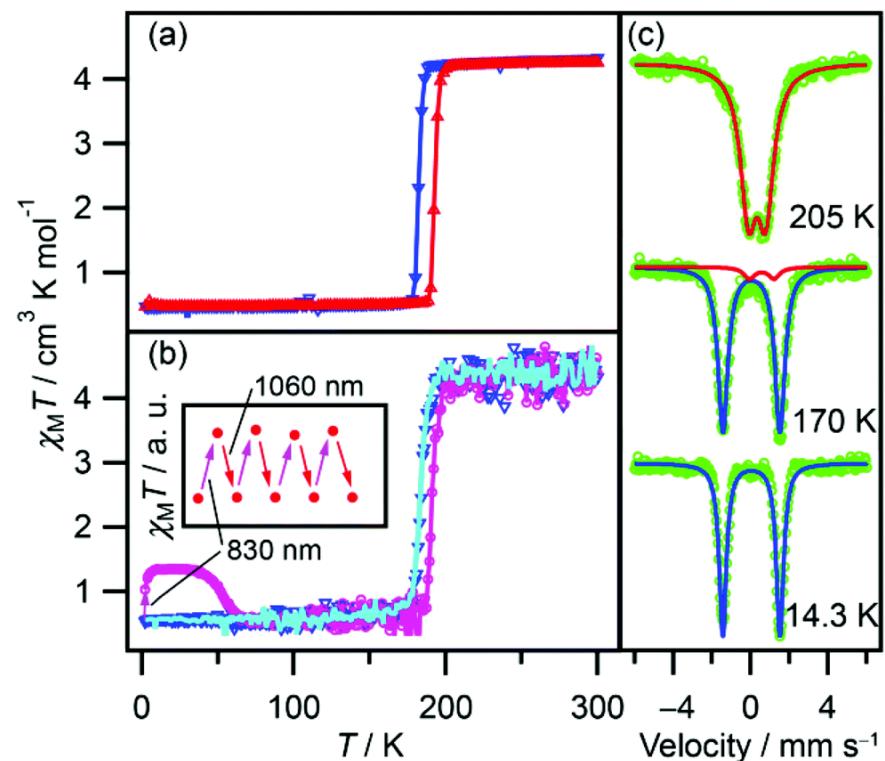
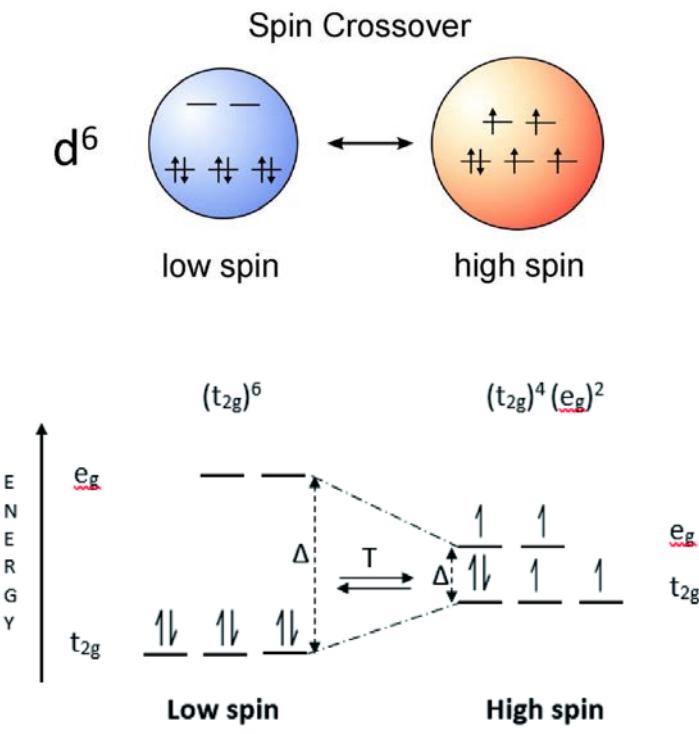
Vysoko a nízkospinové komplexy (HS, LS)



d⁶ HS ... 4 nepárové el. paramagnetický

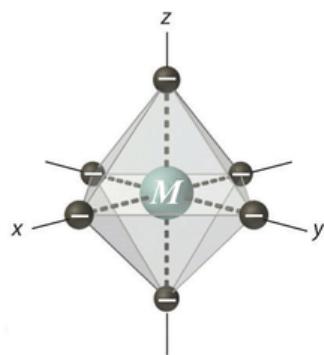
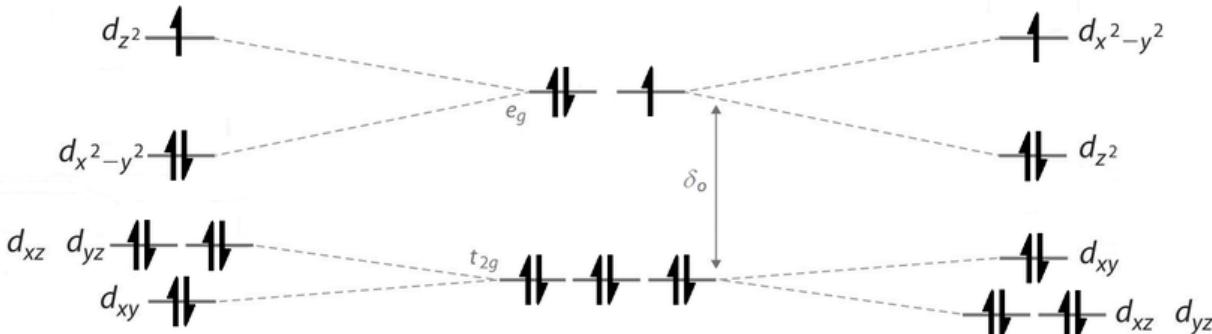
LS ... 0 nepárových el. LS ... 0 nepárových el.

Spin cross over komplexy

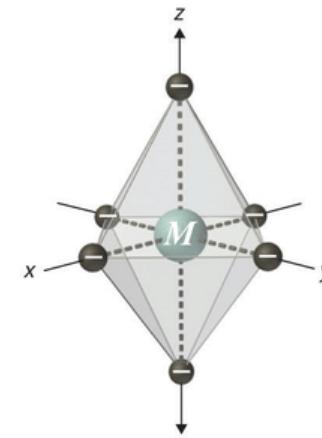


Jahn-Teller

- Degenrované el. konfigurace nejsou stále - spontánní snížení symetrie
- Typické pro d^9

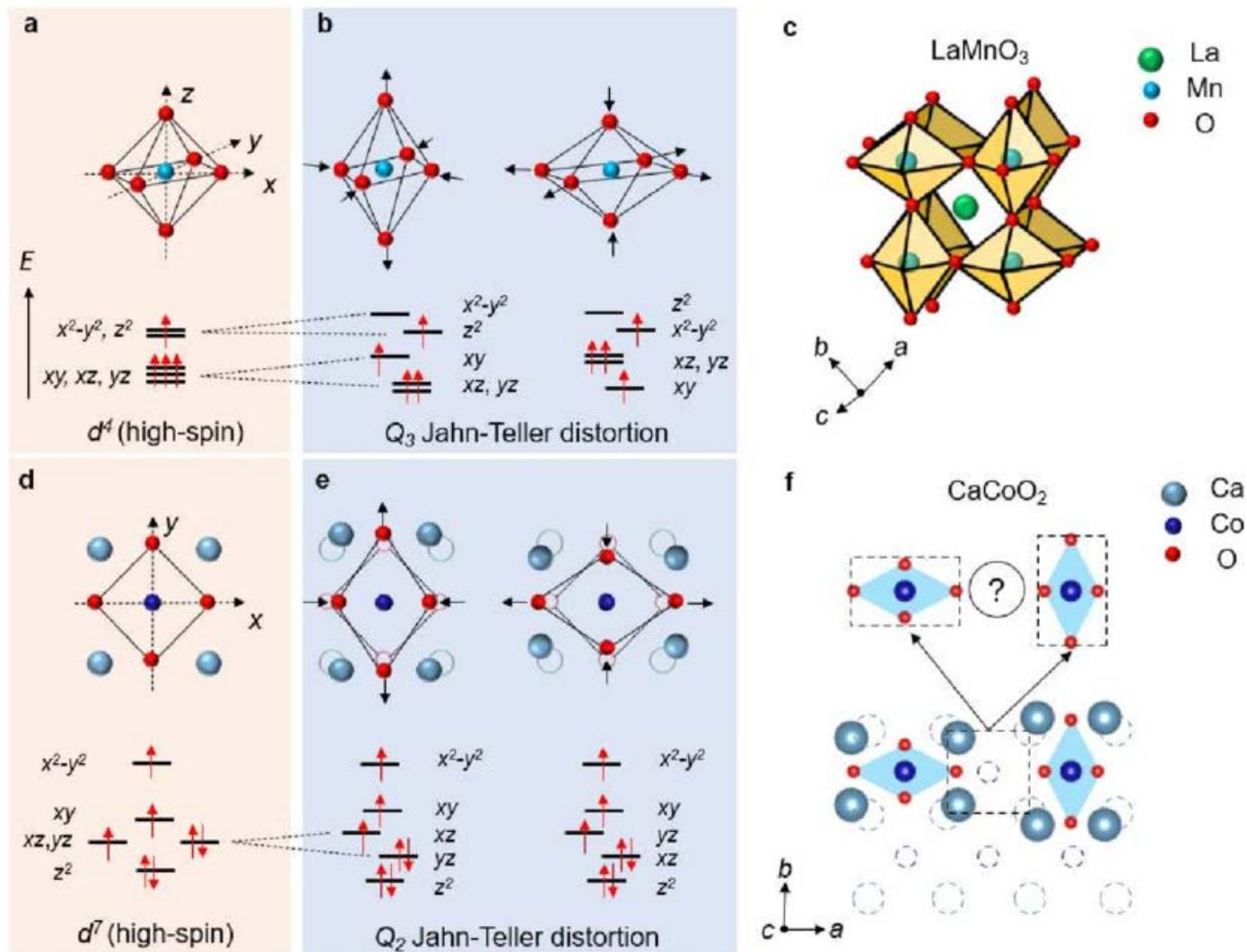


Compressed

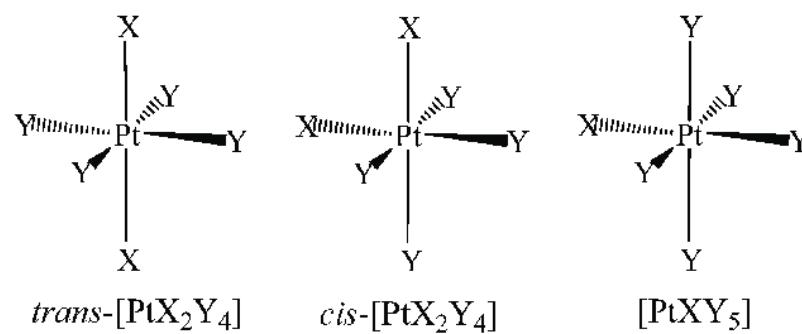
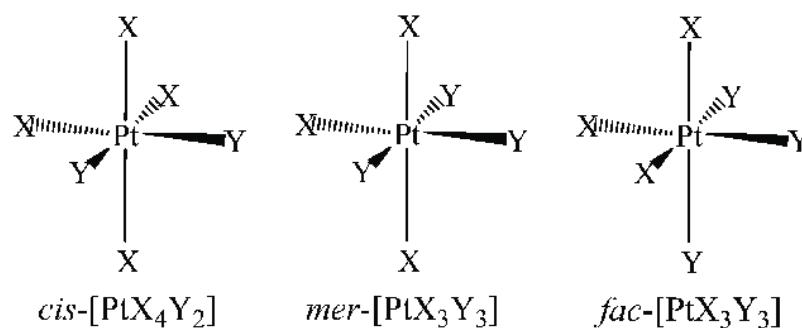
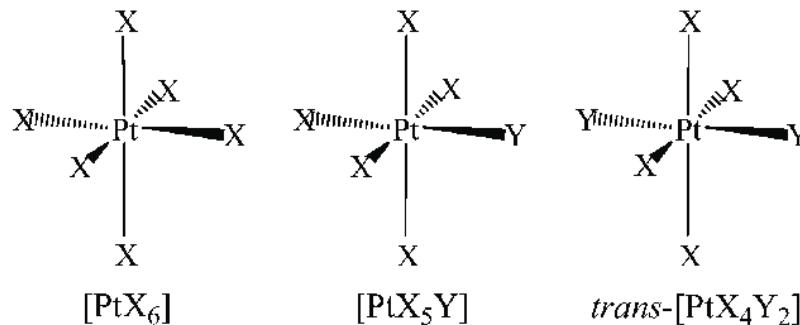


Elongated

Jahn-Teller



Určete prvky, operace a BG symetrie pro sérii komplexů Pt.



Symetrie molekul – bodové grupy

Operace symetrie

je operace, po jejímž provedení je objekt
nerozlišitelný od původního objektu
(transformace molekuly, které nevede k její
zdánlivé změně)

Prvek symetrie

je bod, přímka nebo rovina, vůči které se operace
symetrie provádí

**Ve všech operacích alespoň 1 bod musí
zůstat nezměněn – proto bodové grupy**

Symetrie molekul – bodové grupy

Co je to grupa?

množina G , kde je zavedeno grupové násobení $*$ a platí:

uzavřenost: pro každá a a b z G je $a * b = c$ prvkem G

asociativnost: pro každá a, b, c z G je
 $(a * b) * c = a * (b * c)$

identita: existuje jednotkový prvek e , pro který je
 $a * e = e * a = a$, pro každé a z G

inverze: existuje inverzní prvek, tj. k a z G existuje inverzní prvek a^{-1} , pro který je $a * a^{-1} = a^{-1} * a = e$

Operace bodové symetrie a prvky symetrie

Prvek symetrie	Operace symetrie	Schoenfliesovy symboly	Hermannovy - Mauguinovy symboly
identita	rotace o 360°	E, I	1
n -četná rotační osa	rotace o $2\pi/n$	C_n	n
rovina zrcadlení	zrcadlení	σ	m
střed inverze	inverze	i	$\bar{1}$
n -četná nevlastní osa (rotačně reflexní)	rotace o $2\pi/n$ s zrcadlením v rovině kolmé	$S_1 = \sigma, S_2 = i$ S_n	\tilde{n}
n -četná nevlastní osa (rotačně inverzní)	na rotační osu rotace o $2\pi/n$ následovaná inverzí	C_{ni}	\overline{n}

Multiplikační tabulka grupy

Multiplikační tabulka grupy (C_{2h})

	E	C_2	σ_h	i
E	E	C_2	σ_h	i
C_2	C_2	E	i	σ_h
σ_h	σ_h	i	E	C_2
i	i	σ_h	C_2	E

$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

Maticová reprezentace operací symetrie

$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \cdot \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -x \\ -y \\ -z \end{bmatrix} \quad \mathbf{i} \quad \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \cdot \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x \\ y \\ -z \end{bmatrix} \quad \mathbf{\sigma_{xy}}$$

$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ y_1 \\ z_1 \end{bmatrix} = \begin{bmatrix} -x_1 \\ -y_1 \\ z_1 \end{bmatrix} \quad \mathbf{C}_2$$

$$C_n = \begin{pmatrix} \cos 2\pi/n & \sin 2\pi/n & 0 \\ -\sin 2\pi/n & \cos 2\pi/n & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Obecná rotace

$$S_n = \begin{pmatrix} \cos 2\pi/n & \sin 2\pi/n & 0 \\ -\sin 2\pi/n & \cos 2\pi/n & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Nevlastní rotace

$$\mathbf{C}_n + \mathbf{\sigma_{xy}}$$

Maticové reprezentace

Stejný typ operace symetri – třída – stejný **charakter**:

$$tr(\mathbf{R}') = tr(\mathbf{R})$$

$$\chi(\mathbf{R}') = \chi(\mathbf{R})$$

$$\mathbf{R}' = \mathbf{S}^{-1} \mathbf{R} \mathbf{S}$$

$$\chi(R) = \sum_i D_{ii}(R)$$

$$tr \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = 3$$

Maticové reprezentace operací symetrie – blokové matice – irreducibilní reprezentace

$$\begin{bmatrix} A' & 0 & 0 & 0 \\ 0 & B' & 0 & 0 \\ 0 & 0 & C' \\ 0 & 0 \end{bmatrix} \begin{bmatrix} A'' & 0 & 0 & 0 \\ 0 & B'' & 0 & 0 \\ 0 & 0 & C'' \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} A & 0 & 0 & 0 \\ 0 & B & 0 & 0 \\ 0 & 0 & C \\ 0 & 0 \end{bmatrix}$$

Blok = operace symetrie

Počet irreducibilních reprezentací = počet tříd

$$A'A'' = A$$

$$B'B'' = B$$

$$C'C'' = C$$

Maticové reprezentace



E

$$\chi = 4$$

$$\begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 1 \\ 0 & 1 \end{bmatrix}$$

σ_v

$$\chi = 2$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

C_3^2

$$\chi = 1$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

σ_v

$$\chi = 2$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

C_3

$$\chi = 1$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

$$\begin{array}{l} \mathbf{s}_N \quad \mathbf{s}_1 \quad \mathbf{s}_2 \quad \mathbf{s}_3 \\ \hline \mathbf{s}_N \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \\ \mathbf{s}_1 \begin{bmatrix} 0 & & & \\ & 1 & 0 & 0 \\ & 0 & 1 & 0 \\ & 0 & 0 & 1 \end{bmatrix} \\ \mathbf{s}_2 \begin{bmatrix} 0 & & & \\ & 0 & 1 & 0 \\ & 1 & 0 & 0 \\ & 0 & 0 & 1 \end{bmatrix} \\ \mathbf{s}_3 \begin{bmatrix} 0 & & & \\ & 0 & 0 & 1 \\ & 1 & 0 & 0 \\ & 0 & 1 & 0 \end{bmatrix} \end{array}$$

$$D^{(4)} = D^{(1)} \oplus D^{(3)}$$

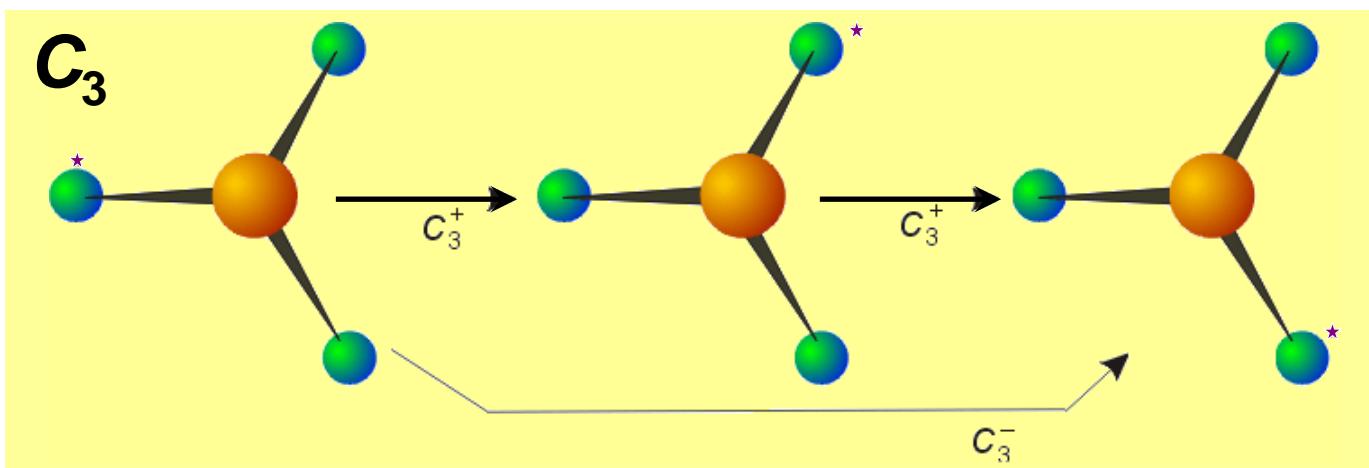
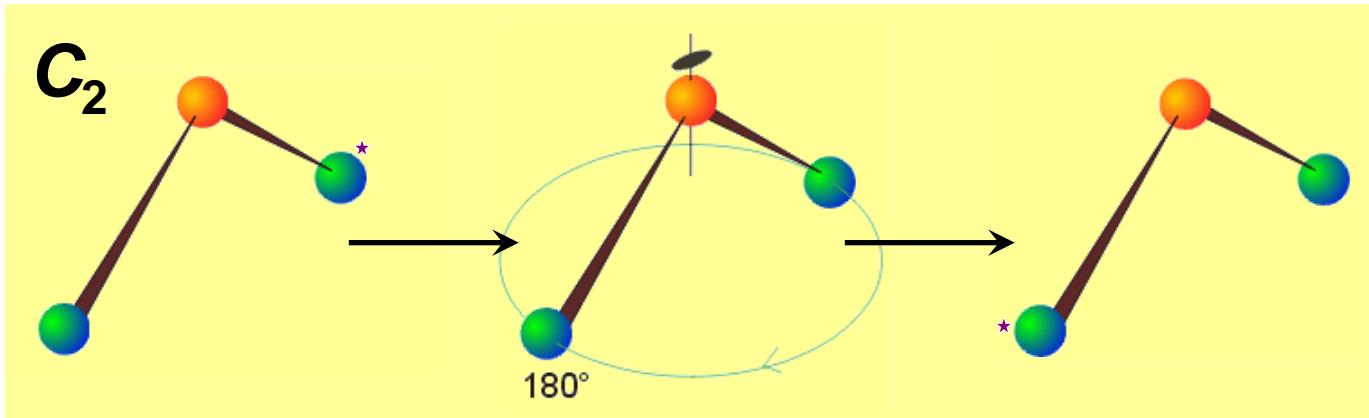
$$D^{(4)} = D^{(1)} \oplus D^{(1)} \oplus D^{(2)}$$

irreducibilní reprezentace

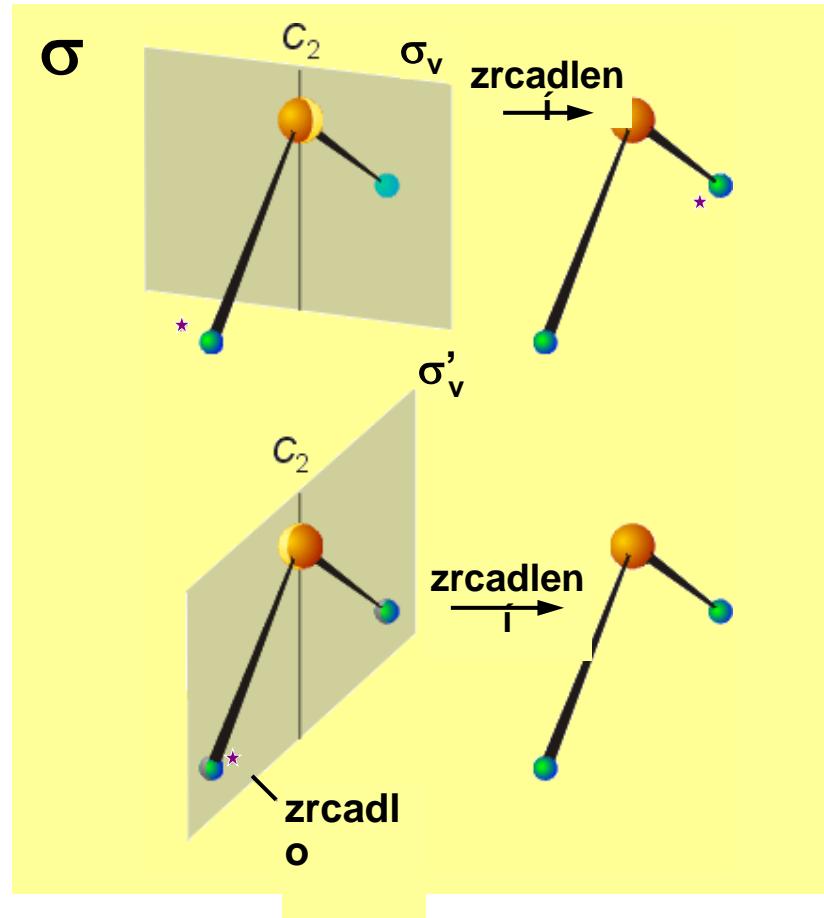
$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Tabelováno! – tabulky charakterů, reflektují multiplikační tabulku BG

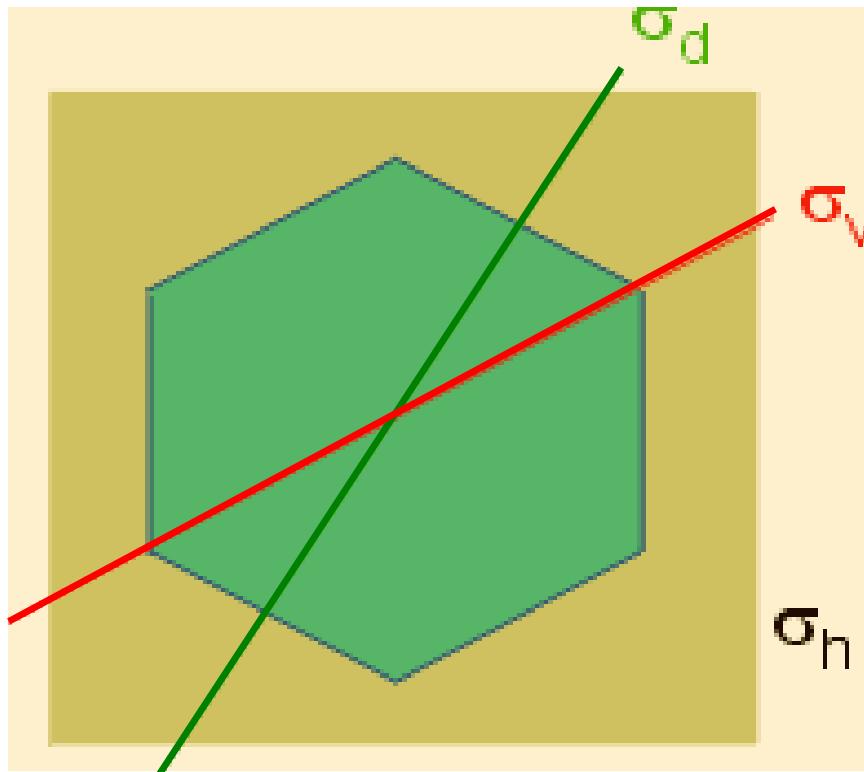
Rotační osy C_n



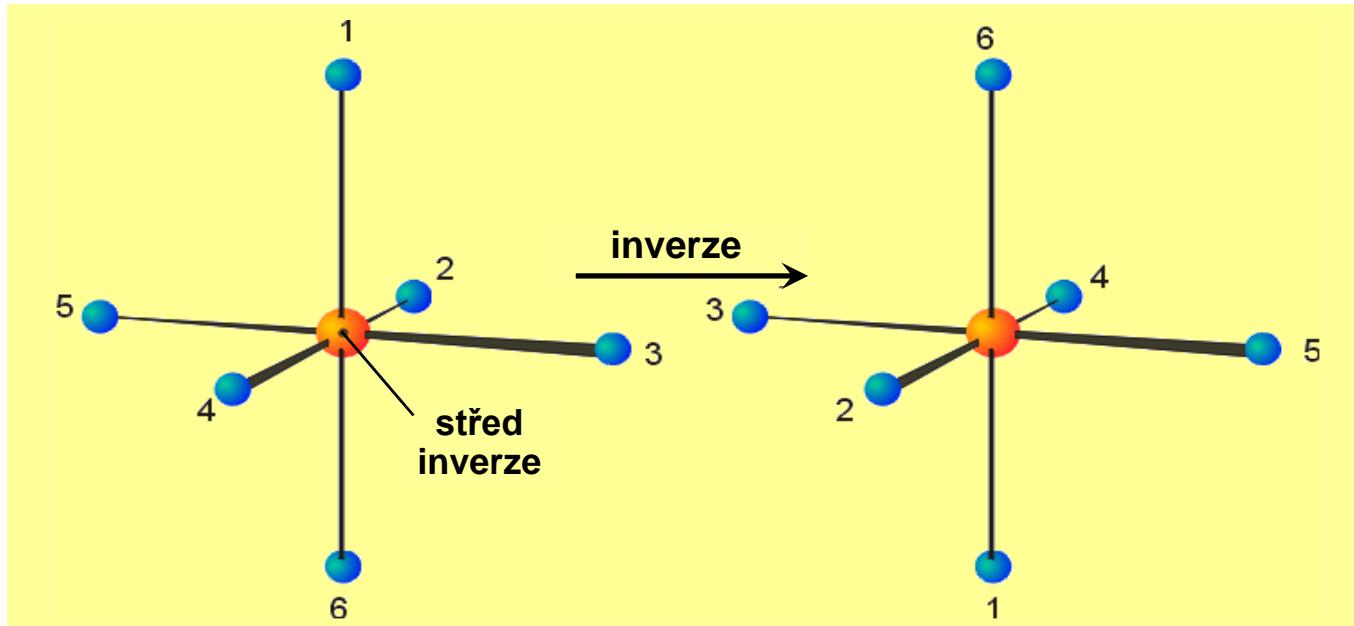
Rovina symetrie σ



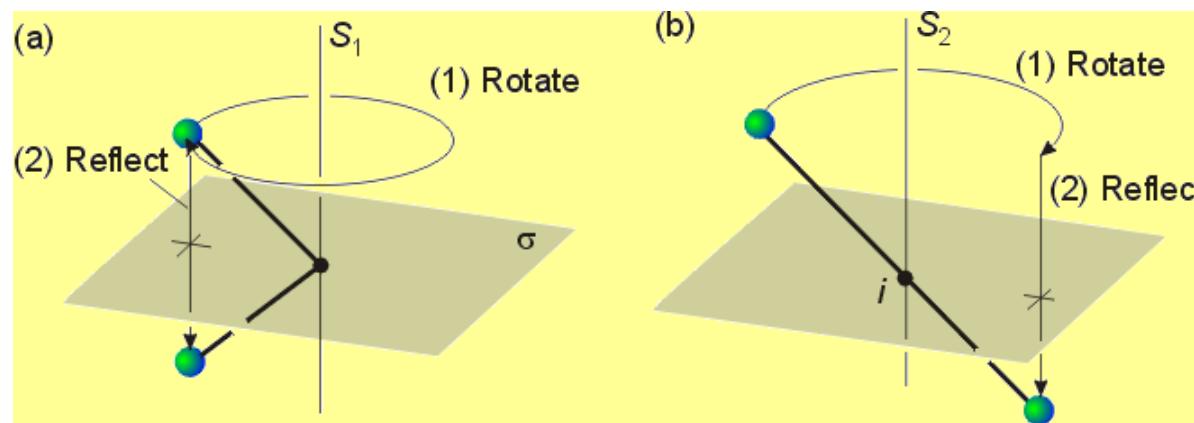
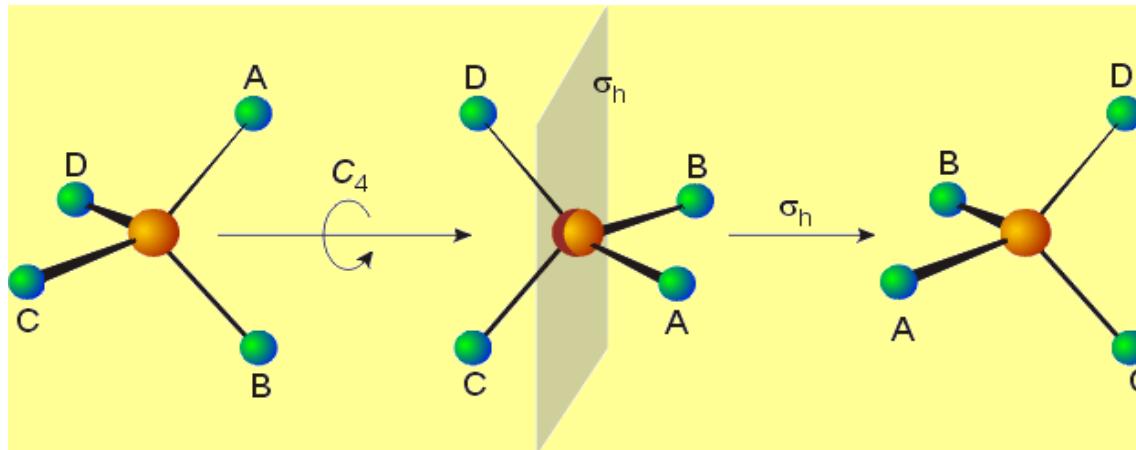
Rovina symetrie σ



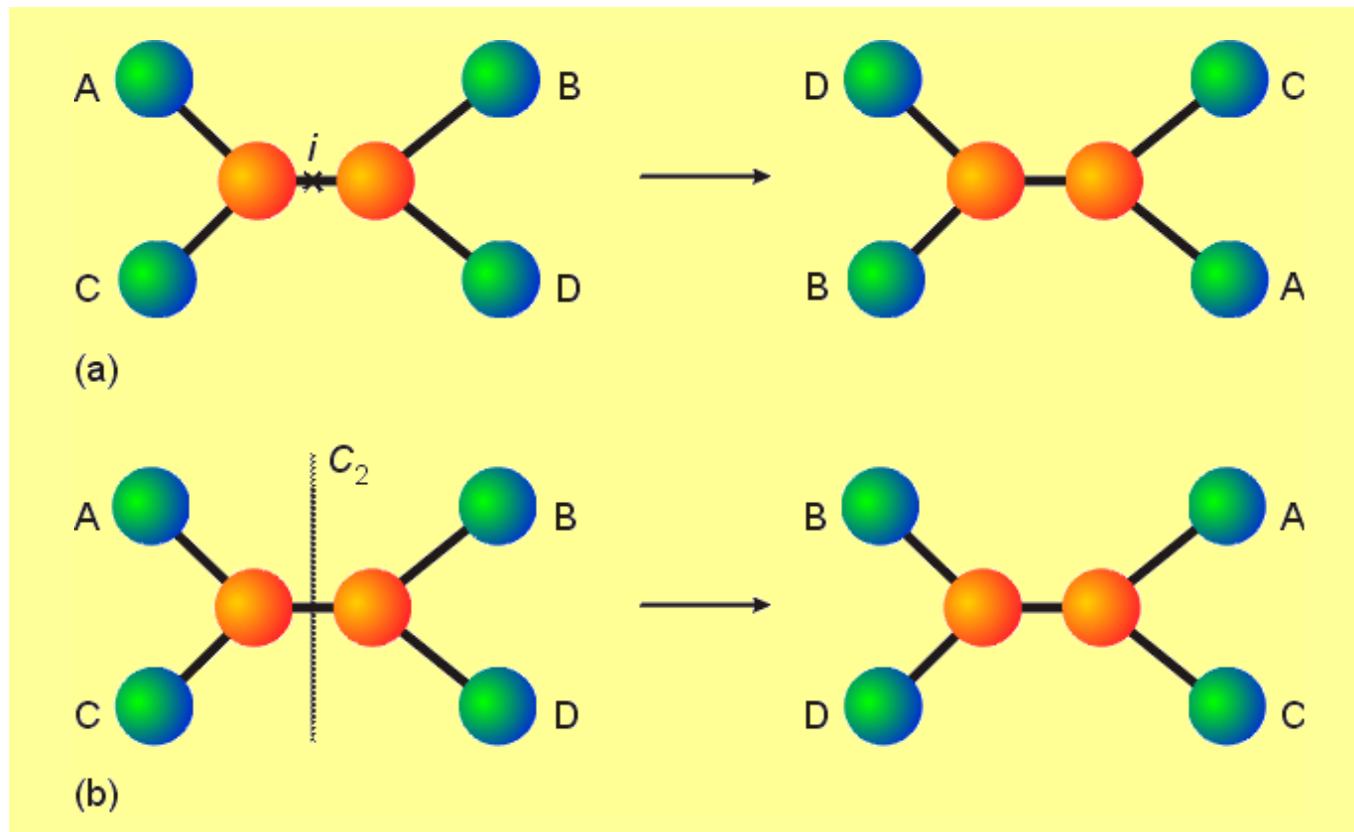
Střed inverze i



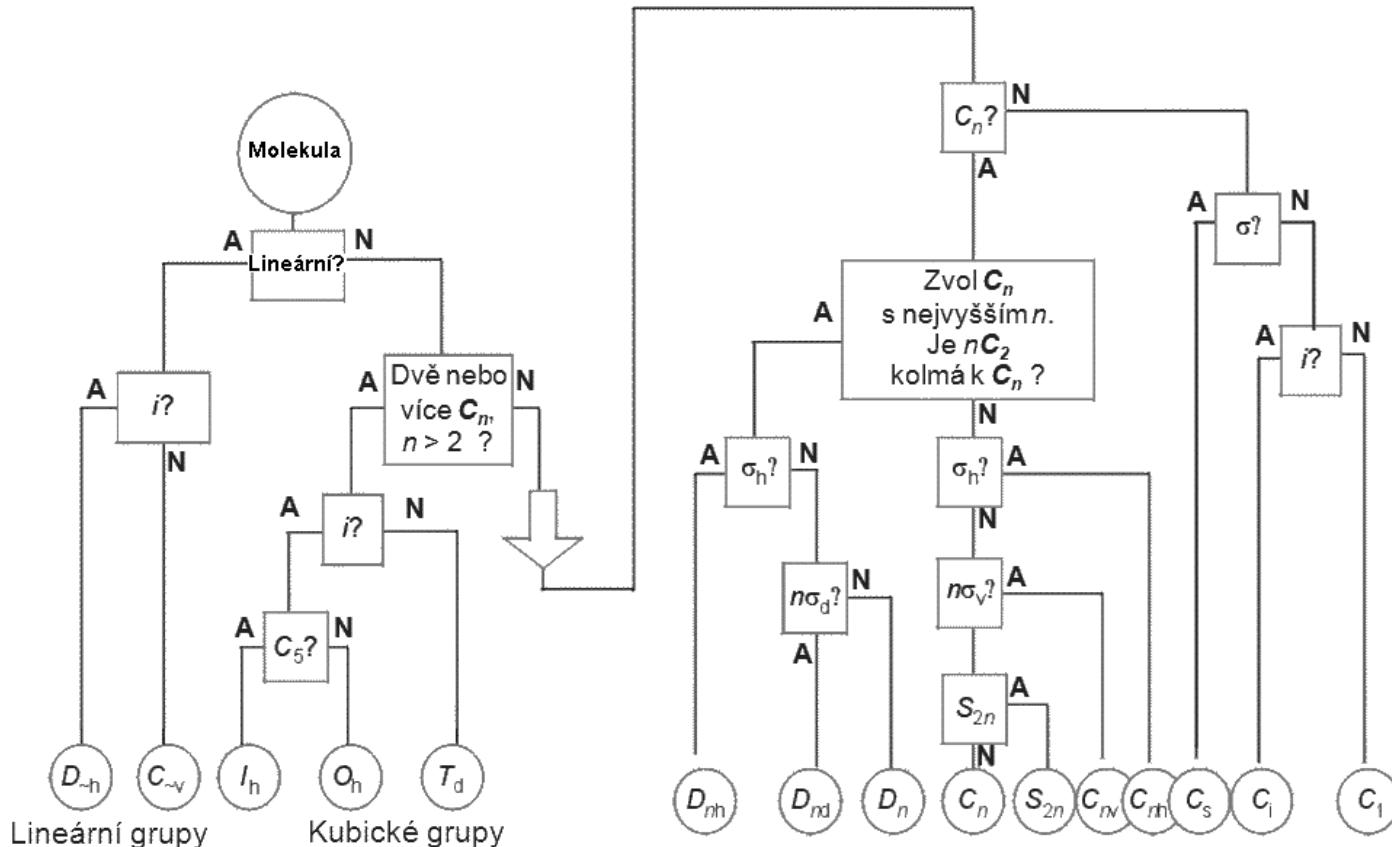
Rotačně reflexní osa S_n



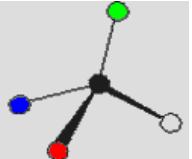
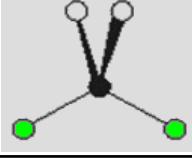
Rotačně inverzní osa C_{ni}



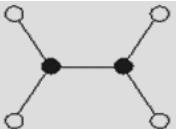
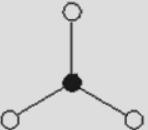
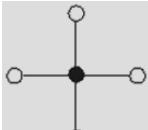
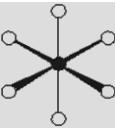
Určení bodových grup symetrie



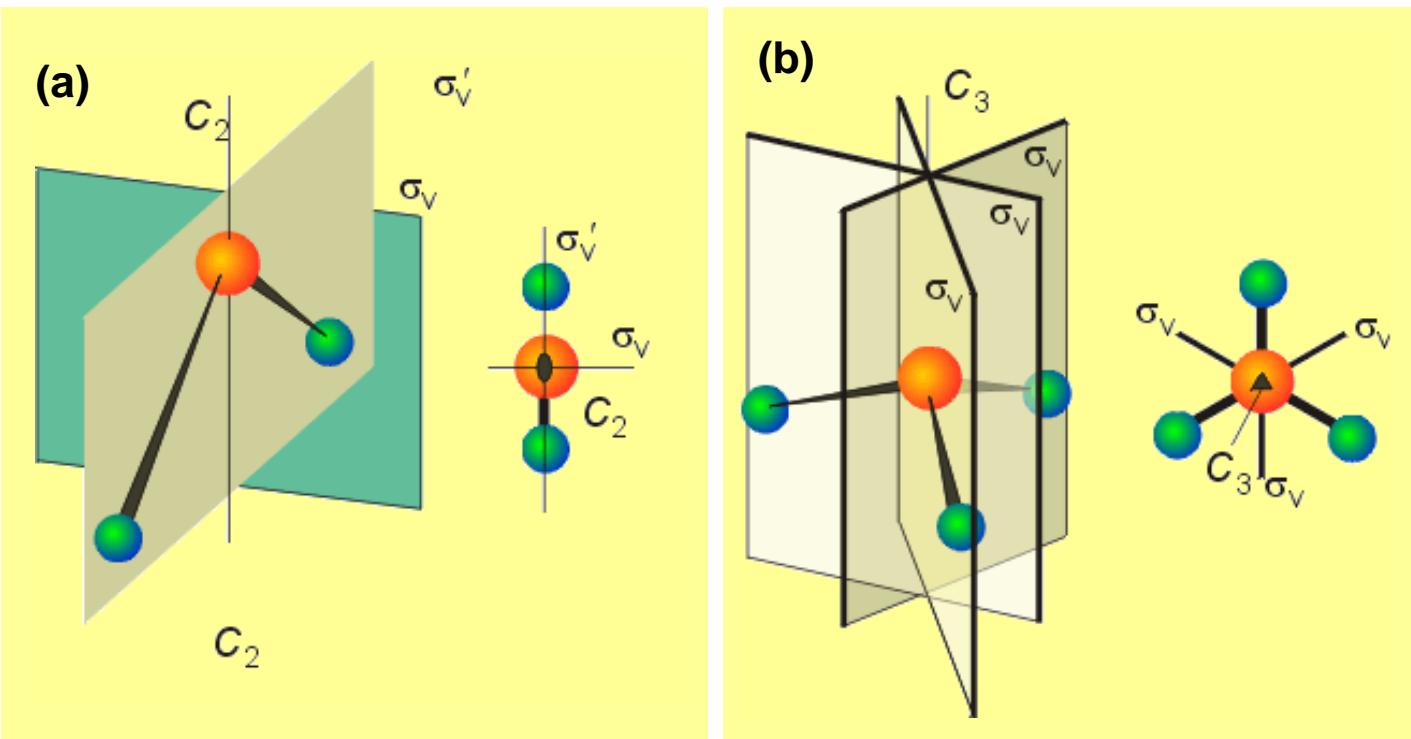
Přehled bodových grup symetrie (1)

BG	Prvky symetrie	Tvar	Příklady
C_1	E		Si Br Cl F I
C_2	E, C_2		H_2O_2
C_s	E, σ		NHF_2
C_{2v}	$E, C_2, \sigma_v, \sigma_v$		SO_2Cl_2, H_2O
C_{3v}	$E, C_3, 3\sigma_v$		$NH_3, PCl_3, POCl_3$
$C_{\infty v}$	$E, C_\infty, \dots \infty \sigma_v$		CO, HCl, OCS

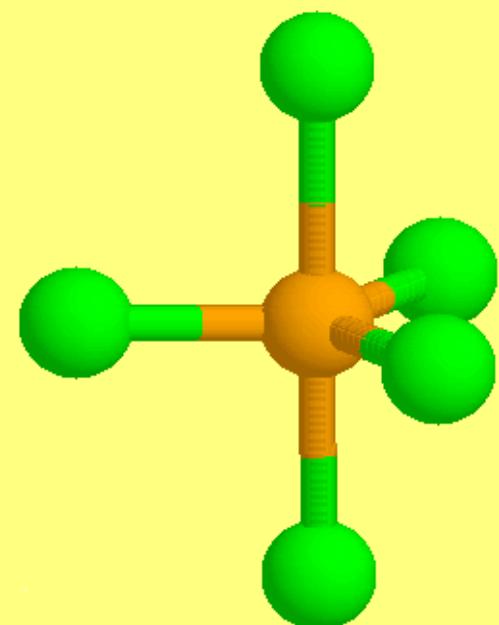
Přehled bodových grup symetrie (2)

BG	Prvky symetrie	Tvar	Příklady
D_{2h}	$E, C_2, (x, y, z), \sigma(xy, yz, zx), i$		N_2O_4, B_2H_6
D_{3h}	$E, C_3, 3C_2, 3\sigma_v, 3\sigma_h, S_3$		BF_3, PCl_5
D_{4h}	$E, C_4, C_2, 2C_2', 2C_2'', i, S_4, \sigma_h, 2\sigma_v, 2\sigma_d$		$XeF_4, trans-MA_4B_2$
$D_{\infty h}$	$E, C_\infty, \dots \infty\sigma_v, i, S_\infty, \dots \infty C_2$		$H_2, CO_2, C_2=H_2$
T_d	$E, 3C_2, 4C_3, 6\sigma_d, 4S_4$		$CH_4, SiCl_4$
O_h	$E, 6C_2, 4C_3, 3C_4, 4S_6, 3S_4, i, 3\sigma_h, 3\sigma_v$		SF_6

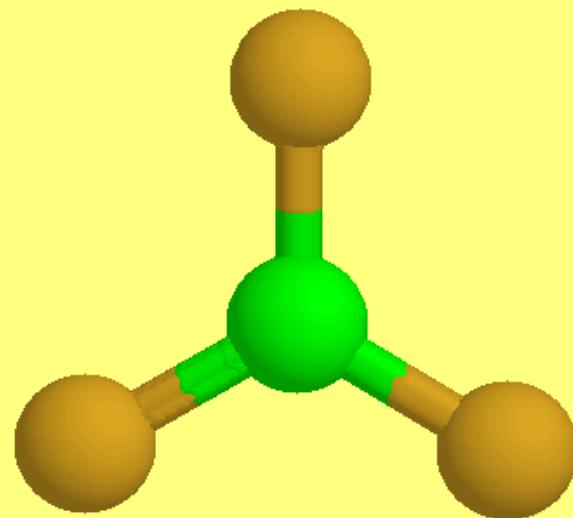
Příklady bodové symetrie (1)



Příklady bodové symetrie (2)

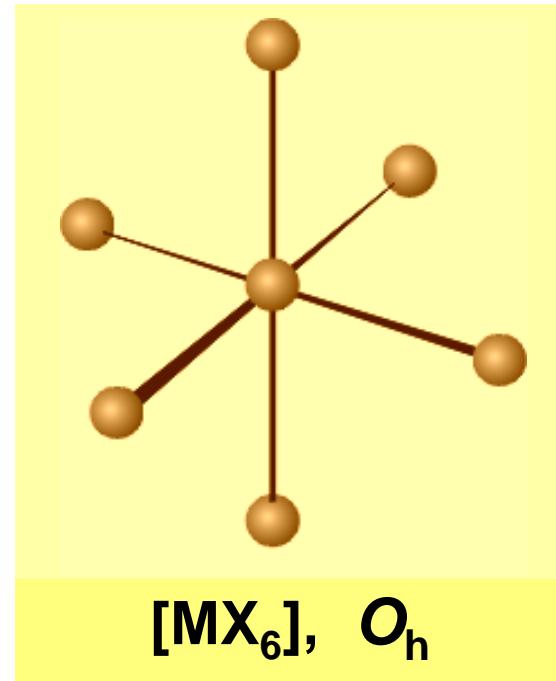
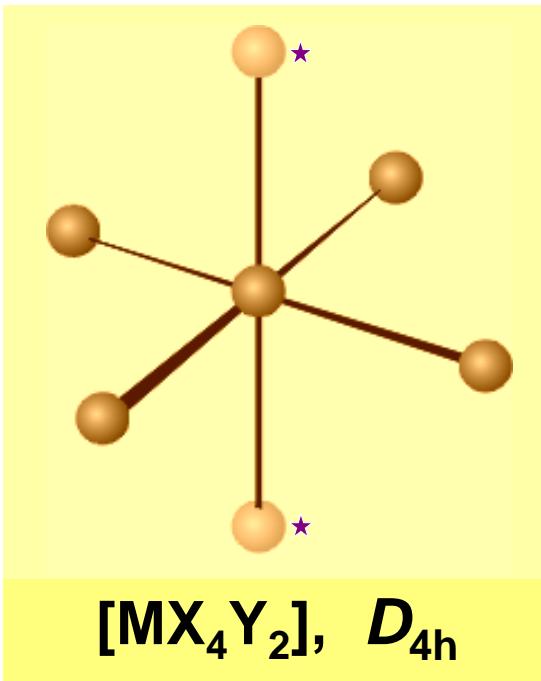
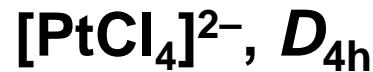
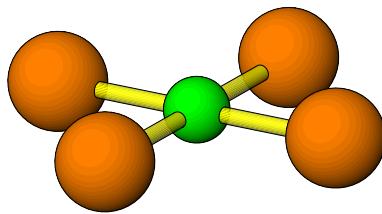


PCl_5, D_{3h}

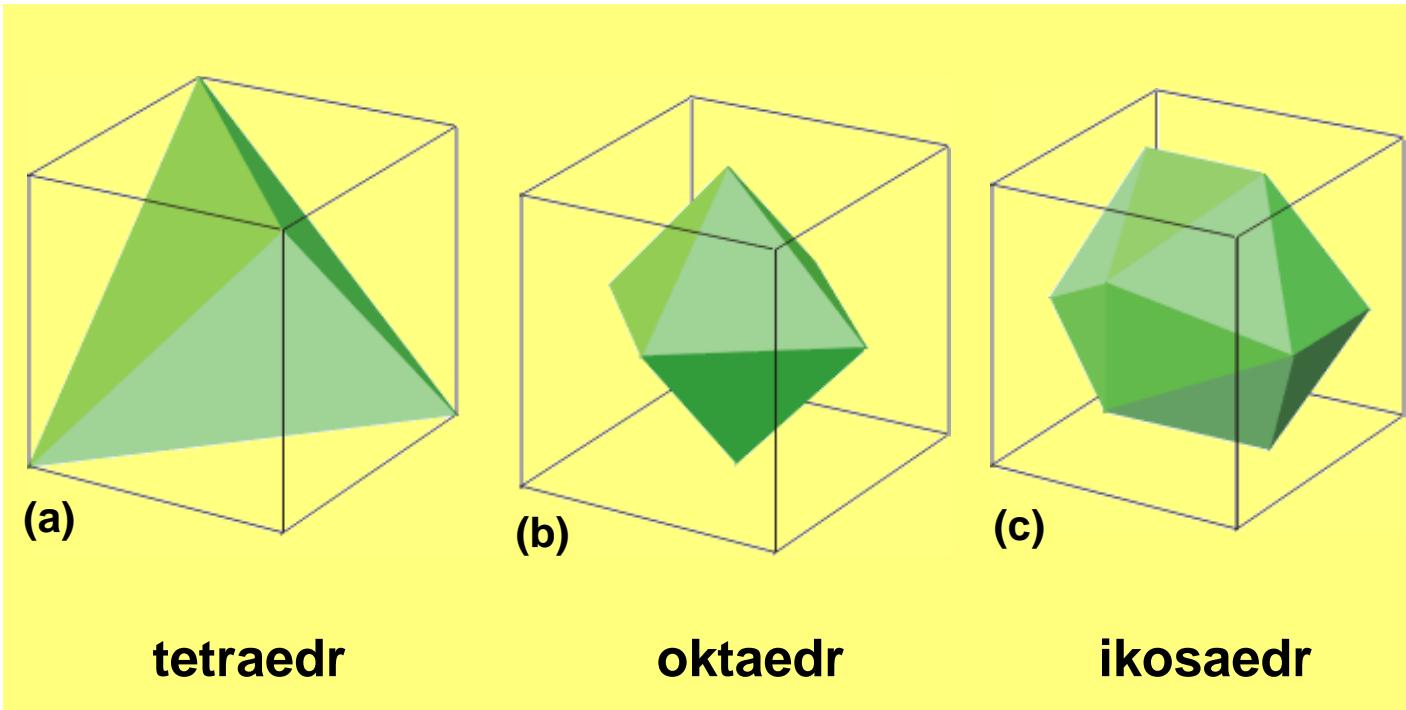


BF_3, D_{3h}

Příklady bodové symetrie (3)



Tělesa s „vyšší“ symetrií



Schoenfliesovy a mezinárodní symboly bodových grup

Soustava	Schoenfliesův symbol	Mezinárodní symbol
triklinická	C_1	1
	C_i	-1
monoklinická	C_2	2
	C_{1h}	m
ortorombická	C_{2h}	2/m
	D_2	222
tetragonální	C_{2v}	mm2
	D_{2h}	2/m 2/m 2/m = mmm
trigonální	C_4	4
	S_4	-4
hexagonální	C_{4h}	4/m
	D_4	422
kubická	C_{4v}	4mm
	D_{2d}	-42m
hexagonální	D_{4h}	4/m 2/m 2/m = 4/mmm
	C_3	3
hexagonální	C_{3i}	-3
	D_3	32
hexagonální	C_{3v}	3m
	D_{3d}	-3 2/m = -3m
hexagonální	C_6	6
	C_{3h}	-6
hexagonální	C_{6h}	6/m
	D_6	622
hexagonální	C_{6v}	6mm
	D_{3h}	-62m
hexagonální	D_{6h}	6/m 2/m 2/m = 6/mmm
	T	23
kubická	T_h	2/m -3 = m-3
	O	432
kubická	T_d	-43m
	O_h	4/m -3 2/m = m-3m

Mullikenova symbolika, reprezentace

<u>Podle symetrie:</u>	hlavní osa rotace (C_n)	střed symetrie (i)	rovina \parallel s hl.osou (σ_v)	rovina \perp k hl.osé (σ_h)
symetrická	A	g	1	'
antisymetrická	B	u	2	"

Závisí na konkrétní grupě

C_2 :

$$\begin{aligned} p_x &\rightarrow -p_x \\ p_y &\rightarrow -p_y \\ \Rightarrow & B \end{aligned}$$

i:

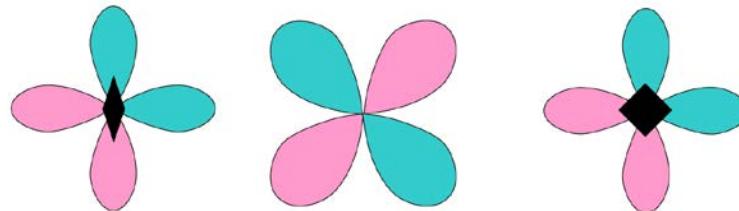
$$\begin{aligned} d_{xy} &\rightarrow d_{xy} \\ (\text{obd. všechny } d) \\ \Rightarrow & g \end{aligned}$$

C_4 :

$$\begin{aligned} p_x &\rightarrow p_y \\ p_y &\rightarrow -p_x \\ \Rightarrow & E \end{aligned}$$

Podle degenerace:

- 1: A,B
- 2: E
- 3: T



Symbolika irreducibilních reprezentací

C_{2v} (2mm)	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$	$h = 4$
A_1	1	1	1	1	z
A_2	1	1	-1	-1	R_z
B_1	1	-1	1	-1	x, R_y
B_2	1	-1	-1	1	y, R_x

Pro degenerované orbitaly je charakter reprezentace roven součtu charakterů odpovídajících jednotlivým orbitalům, které po transformaci zůstávají na původním místě, nebo mění jen své znaménko.

C_{2h}	E	C_2	σ_h	i	$h=4$
A_g	1	1	1	1	R_z
A_u	1	1	-1	-1	z
B_g	1	-1	-1	1	R_x, R_y
B_u	1	-1	1	-1	x, y

Suma druhých mocnin degenerací jednotlivých reprezentací je rovna řádu grupy ($h=\sum n^2$ tj. $4=1^2+1^2+1^2+1^2$)
Počet reprezentací je roven počtu tříd grupy.

Symbolika irreducibilních reprezentací

	C_n	i	σ_v	σ_h
symetrická	A	g	1	v
antisymetrická	B	u	2	w

O_h (m3m)	E	$8C_3$	$6C_2$	$6C_4$	$3C_2$ (= C_4^2)	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$	$h = 48$
A_{1g}	1	1	1	1	1	1	1	1	1	1	$x^2 + y^2 + z^2$
A_{2g}	1	1	-1	-1	1	1	-1	1	1	-1	
E_g	2	-1	0	0	2	2	0	-1	2	0	$(2z^2 - x^2 - y^2, x^2 - y^2)$
T_{1g}	3	0	-1	1	-1	3	1	0	-1	-1	(R_{xz}, R_{yz}, R_z)
T_{2g}	3	0	1	-1	-1	3	-1	0	-1	1	(xz, yz, xy)
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1	
A_{2u}	1	1	-1	-1	1	-1	1	-1	-1	1	
E_u	2	-1	0	0	2	-2	0	1	-2	0	
T_{1u}	3	0	-1	1	-1	-3	-1	0	1	1	(x, y, z)
T_{2u}	3	0	1	-1	-1	-3	1	0	1	-1	