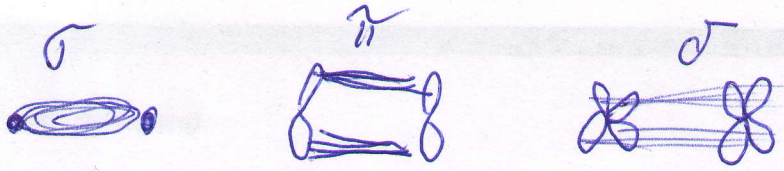
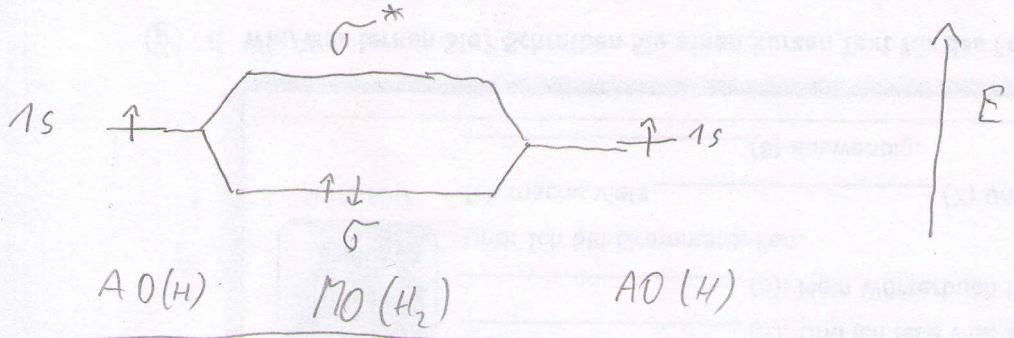
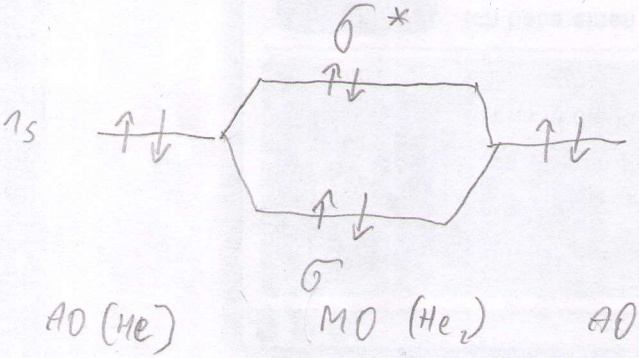


MO - LCAO

Řád vazby: $\check{R}V = \frac{\text{vazebné } e^{\ominus} - \text{protivazebné } e^{\ominus}}{2}$

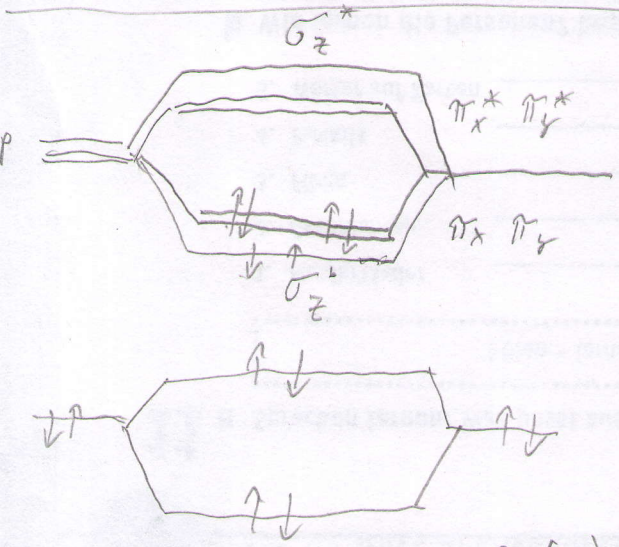
větší řád – větší vaz. E (pevnější vazba)
– kratší vazebná vzdálenost.

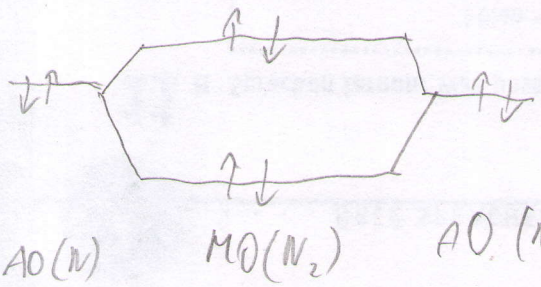




$\check{R}V = 0$

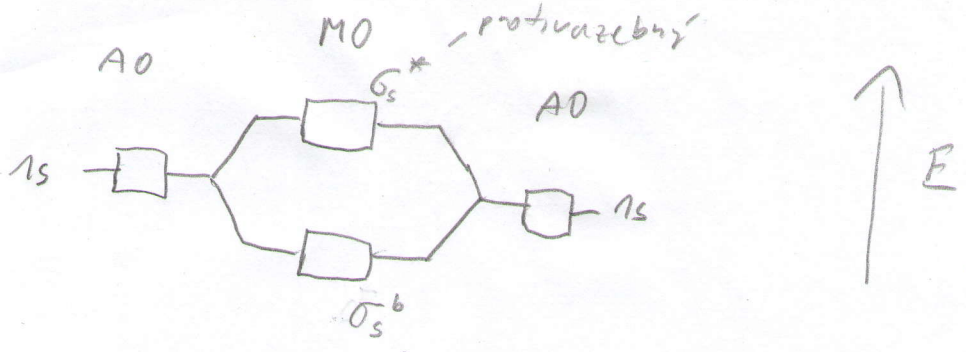
He_2 netvoří dvouatom. molekuly

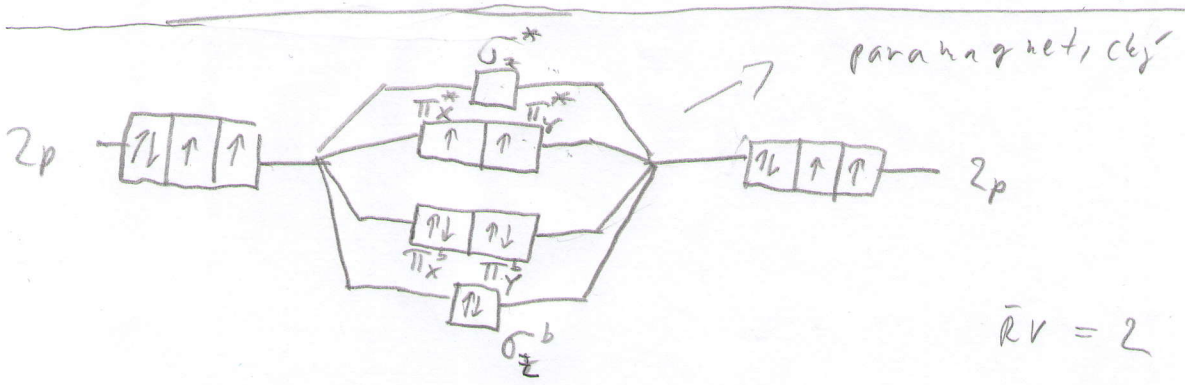




$\check{R}V = 3$

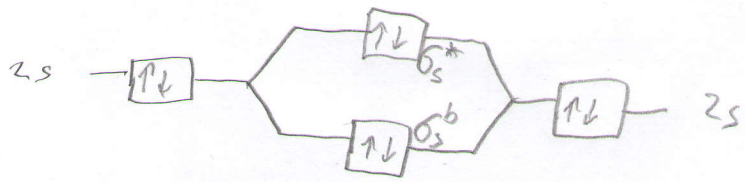
$N \equiv N$

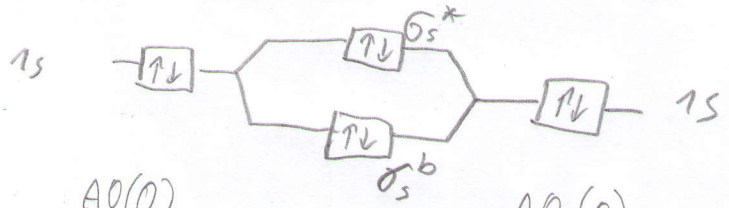




$\bar{R}V = 2$

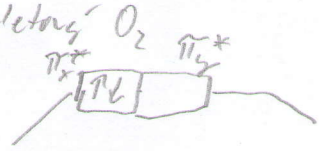
$O = O$





tripletový O_2

singletový O_2

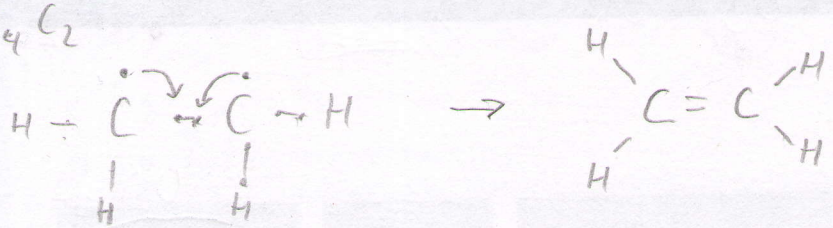


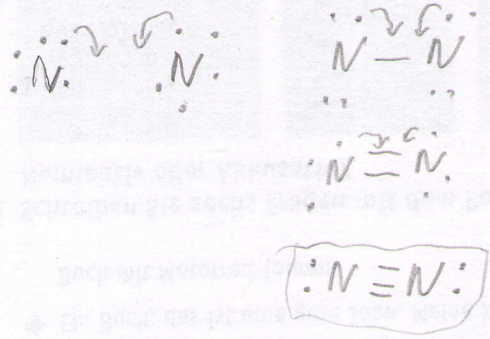
HOMO/LUMO - nejvyšší obsazený a nejnižší neobsazený MO. Energetický rozdíl charakterizuje schopnost excitace molekuly

- látka obsahující atomy nebo molekuly s nespárovanými e^- je paramagnetická (chová se jako slabý magnet, je slabě vtahována do vnějšího mag. pole)

Oktetové pravidlo

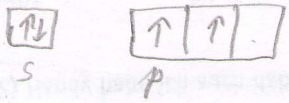
H_4C_2





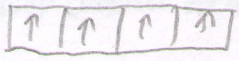
Hybridizace

$C: [He]\ 2s^2\ 2p^2$

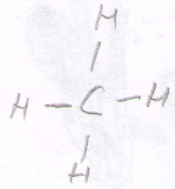


$C^*_{excit.}$

C



sp^3



Hybridizace	Geometrie molekuly	úhel
sp	lineární	180°
sp^2	trojúhelník	120°
sp^3	tetraedr	109,5°
sp^2d	čtverec	90°
sp^3d^2	oktaedr	90°
sp^3d	trigonální bipyramida	120° a 90°

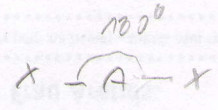
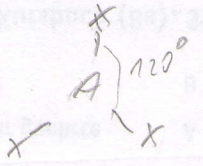
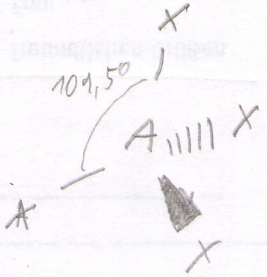
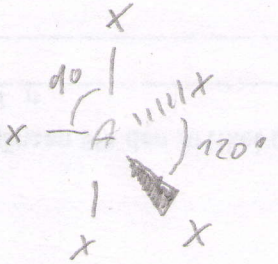
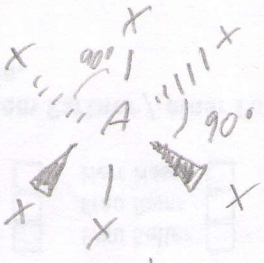
VSEPR

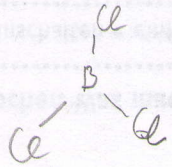
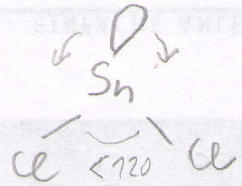
- el. páry se rozmístí, aby měly nejnižší E

- nevazebný el. pár

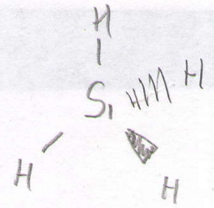
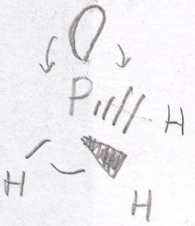
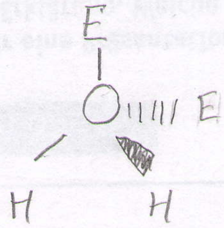
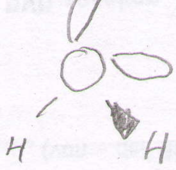
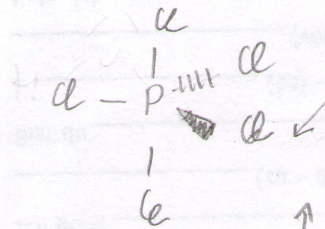
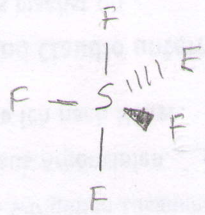
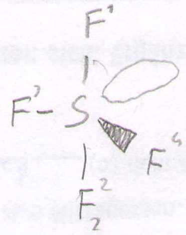
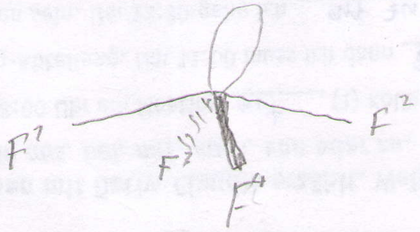
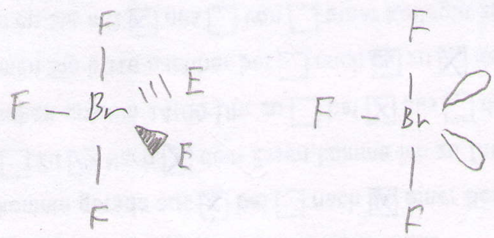
odpuzování: nevazebný ē pár > trojná vazba > dvojná vazba > jednoduchá vazba

- tvar molekuly je dán pouze polohou vazebných ē párů

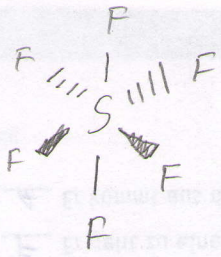
ē páry	tvar	úhly	
2	lineární	180	
3	trojúhelník	120	
4	tetraedr	109,5	
5	trigonální bipyramida		
6	oktaed		

		typ	úhel	tvar molekuly
CO_2	O = C = O	AX_2	180	lineární
CO	⬭ C=O	AXE	180	lineární
BCl_3		AX_3	120	trojúhelník
$SnCl_2$		AX_2E	<120	lomená struktura

lomená struktura

SiH_4		AX_4	$109{,}5°$	tetraedr
PH_3		AX_3E	$<109{,}5°$	trigonální pyramida
H_2O	 	AX_2E_2	$<109{,}5°$	lomená struktura
PCl_5	 ekvatoriální rovina; axiální rovina	AX_5	$120°$; $90°$	trigonální bipyramida
SF_4	 	AX_4E	$<120°$, $<90°$	houpačka
BrF_3		AX_3E_2	$<90°$	tvar T
XeF_2		AX_2E_3	$180°$	lineární

SF_6

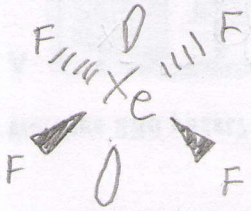


AX_6 90° Oktaedr

IF_5

AX_5E <90° čtvercová pyramida

XeF_4



AX_4E_2 90° čtverec