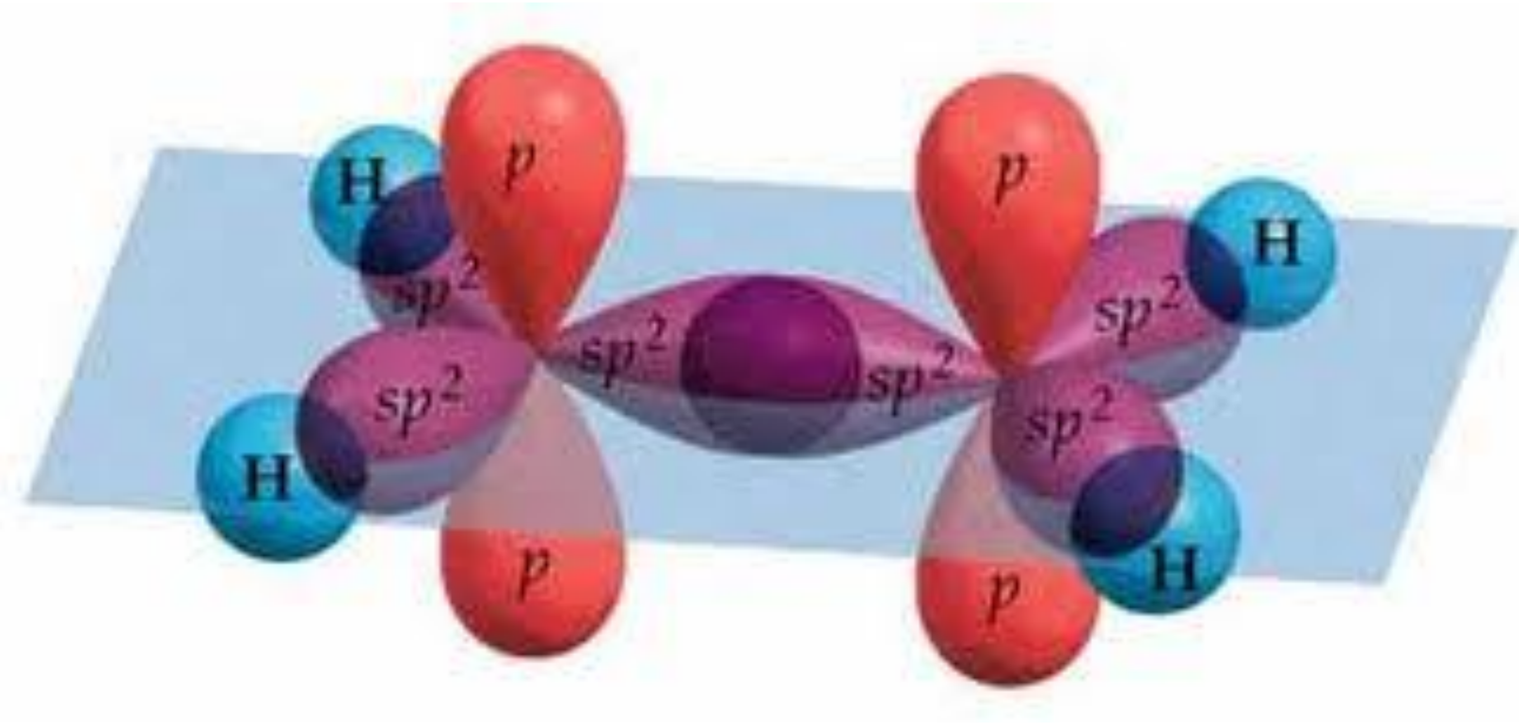
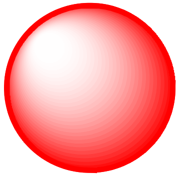
Obecná chemie uhlíku a vodíku, orbitaly, hybridizace, vazby, typy reakcí, kinetika a termodynamika

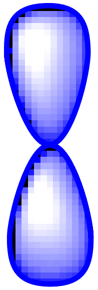
Teorie orbitalů a vazeb



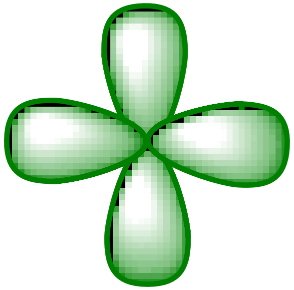
Atomové orbitaly



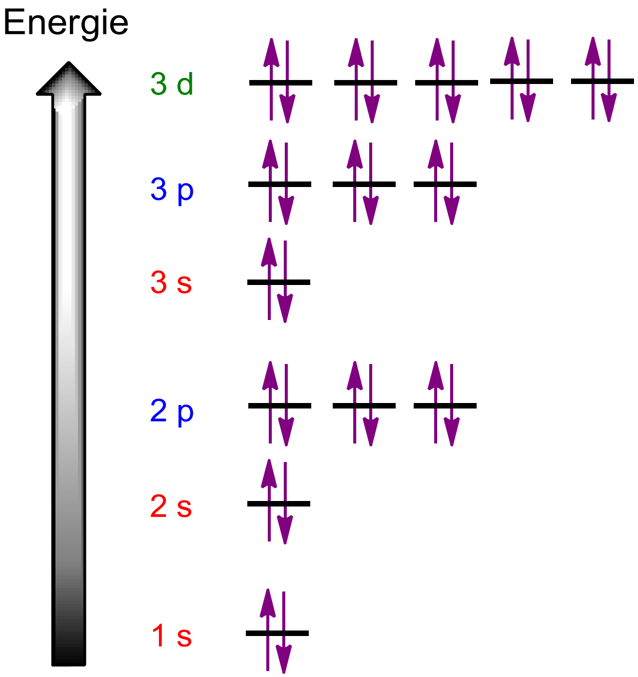
orbital s



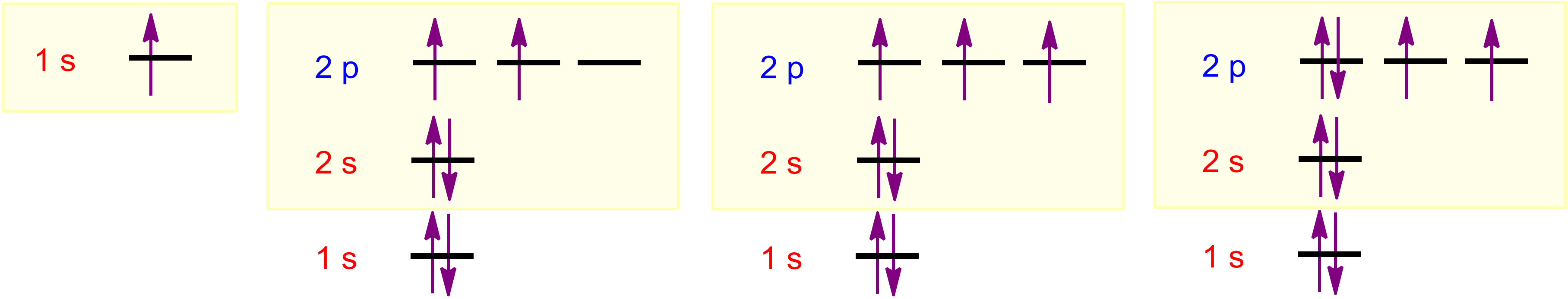
orbital p



orbital d



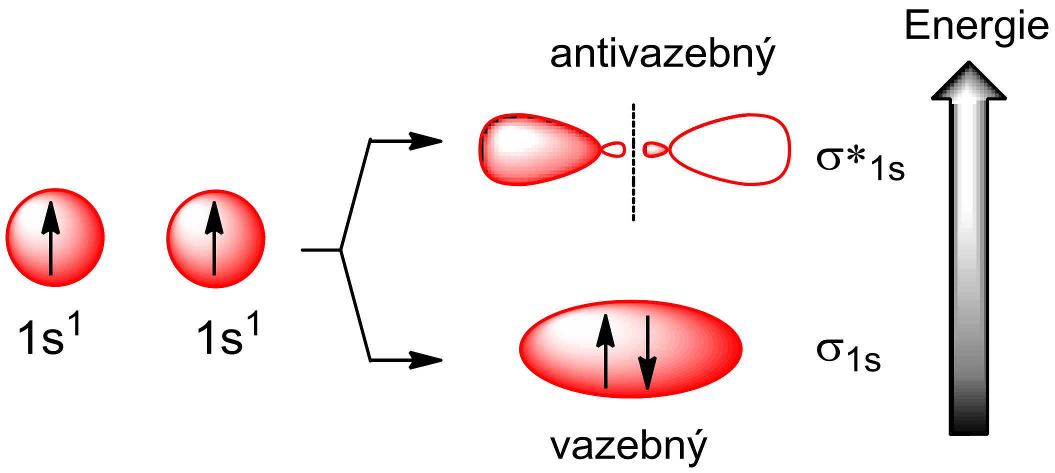
Elektronové konfigurace vybraných prvků



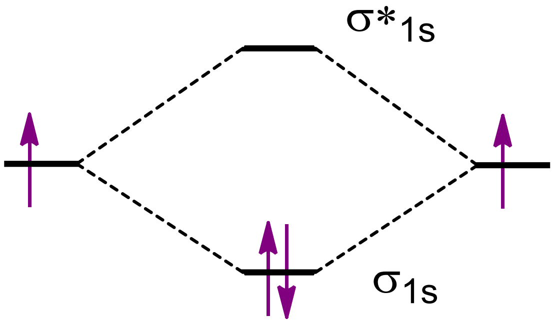
Vodík ^{1}**H**	**Uhlík** ^{12}**C**	**Dusík** ^{14}**N**	**Kyslík** ^{16}**O**
1 elektron	6 elektronů	7 elektronů	8 elektronů
$\mathbf{1s^{1}}$	$\mathbf{1s^{2}2s^{2}2p_{x}^{1}2p_{y}^{1}}$	$\mathbf{1s^{2}2s^{2}2p_{x}^{1}2p_{y}^{1}2p_{z}^{1}}$	$\mathbf{1s^{2}2s^{2}2p_{x}^{2}2p_{y}^{1}2p_{z}^{1}}$
1 valenční elektron	4 valenční elektrony	5 valenčních elektronů	6 valenčních elektronů

Molekulové orbitaly - molekula H_2

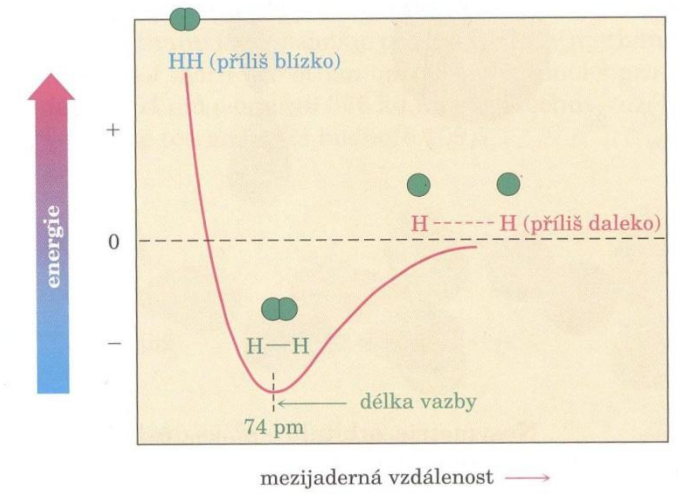
atomové orbitaly **molekulové orbitaly**

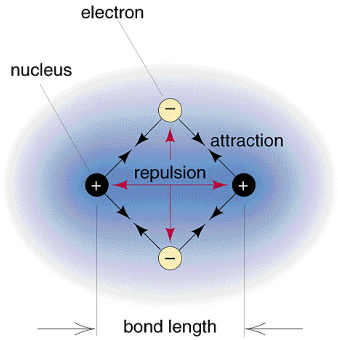


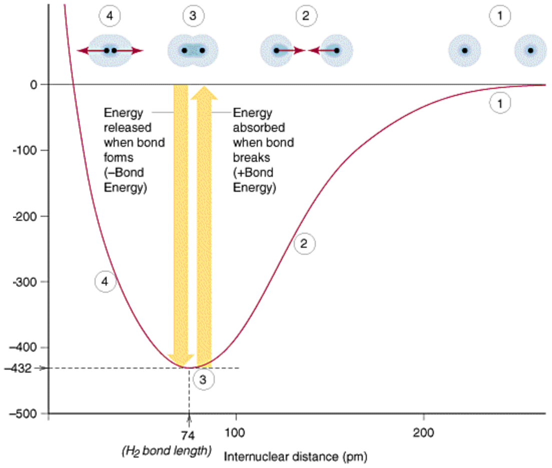
LUMO - lowest unoccupied molecular orbital



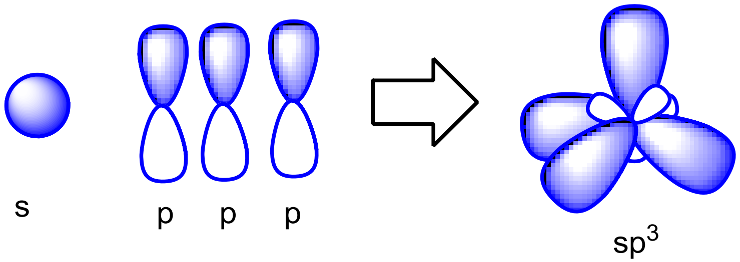
HOMO - highest occupied molecular orbital

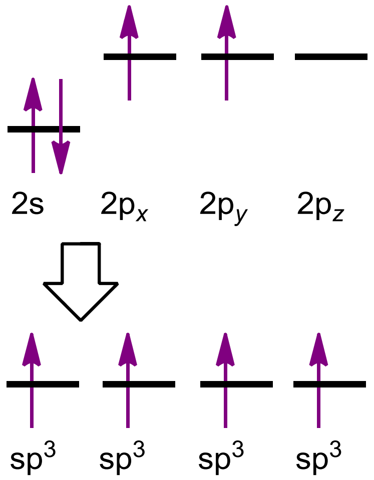


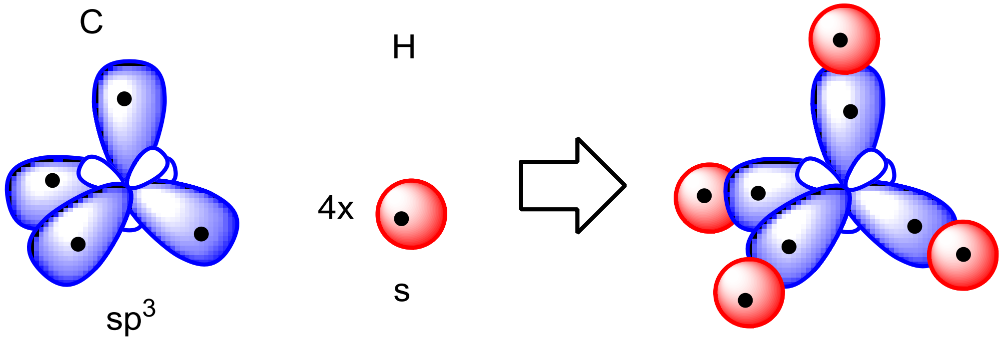


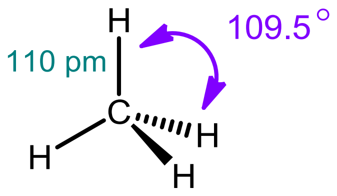


Molekulové orbitaly – hybridizace C

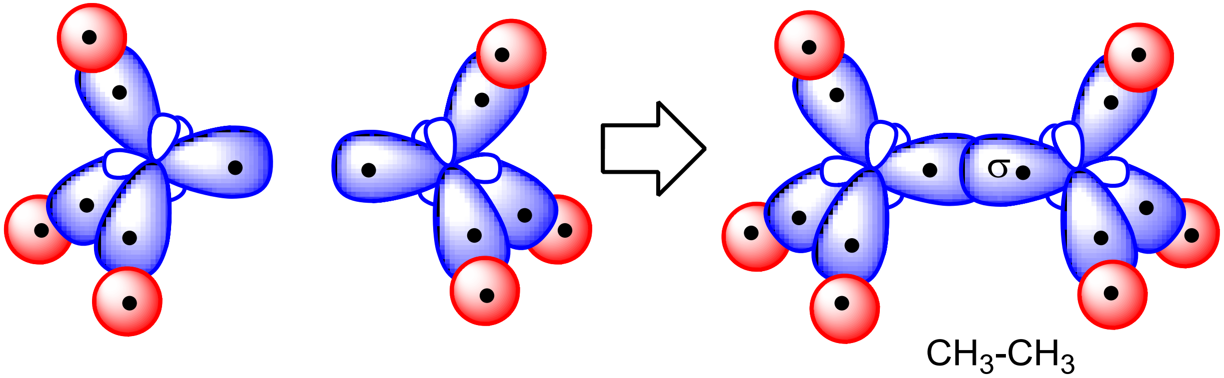




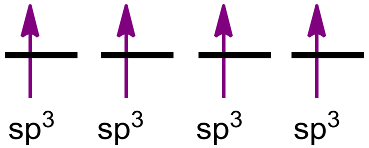


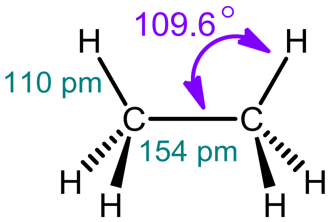


Molekulové orbitaly – jednoduchá vazba C-C, molekula ethanu

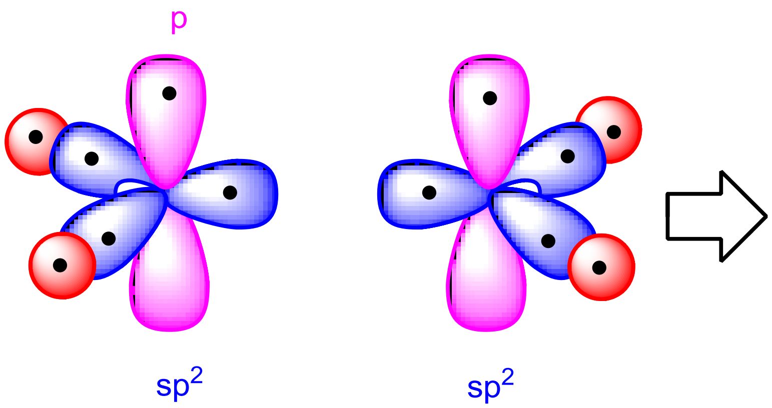


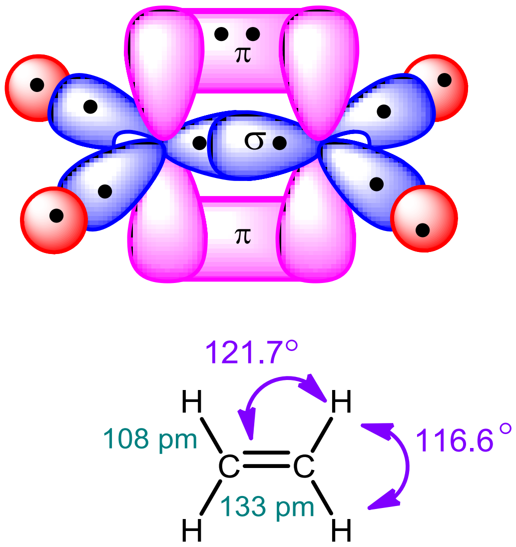
sp^3

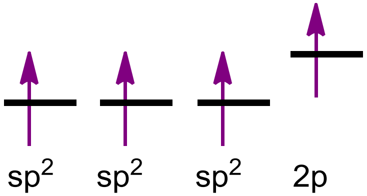




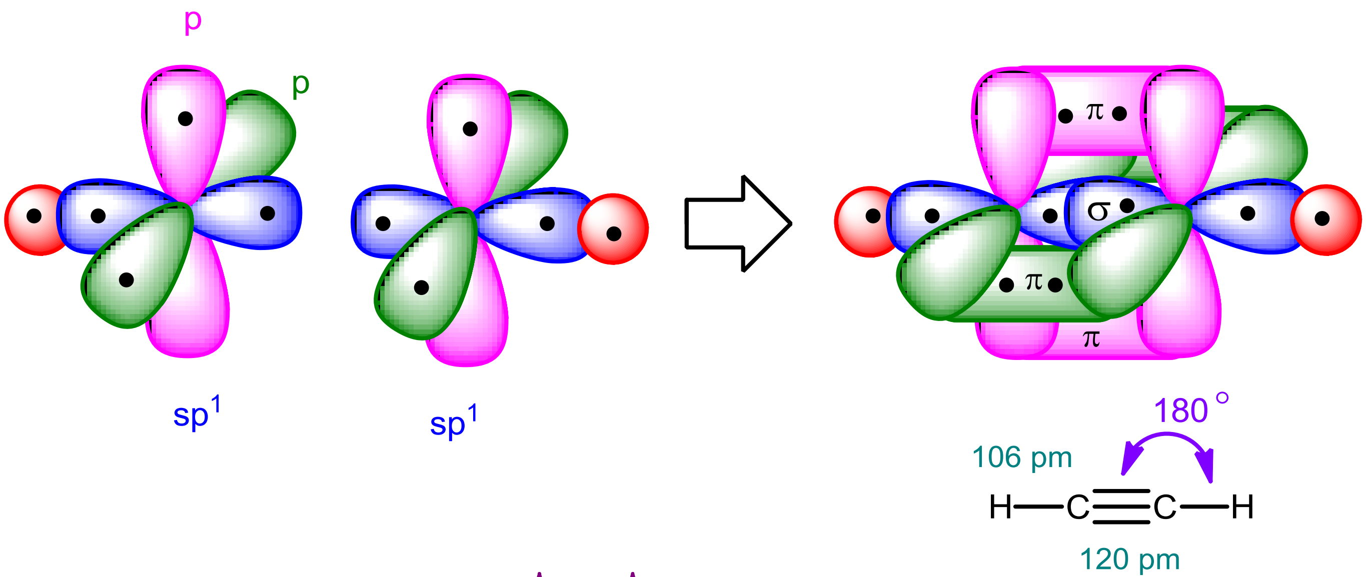
Molekulové orbitaly – dvojná vazba C=C, molekula ethenu

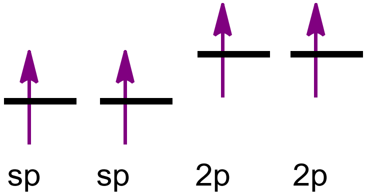


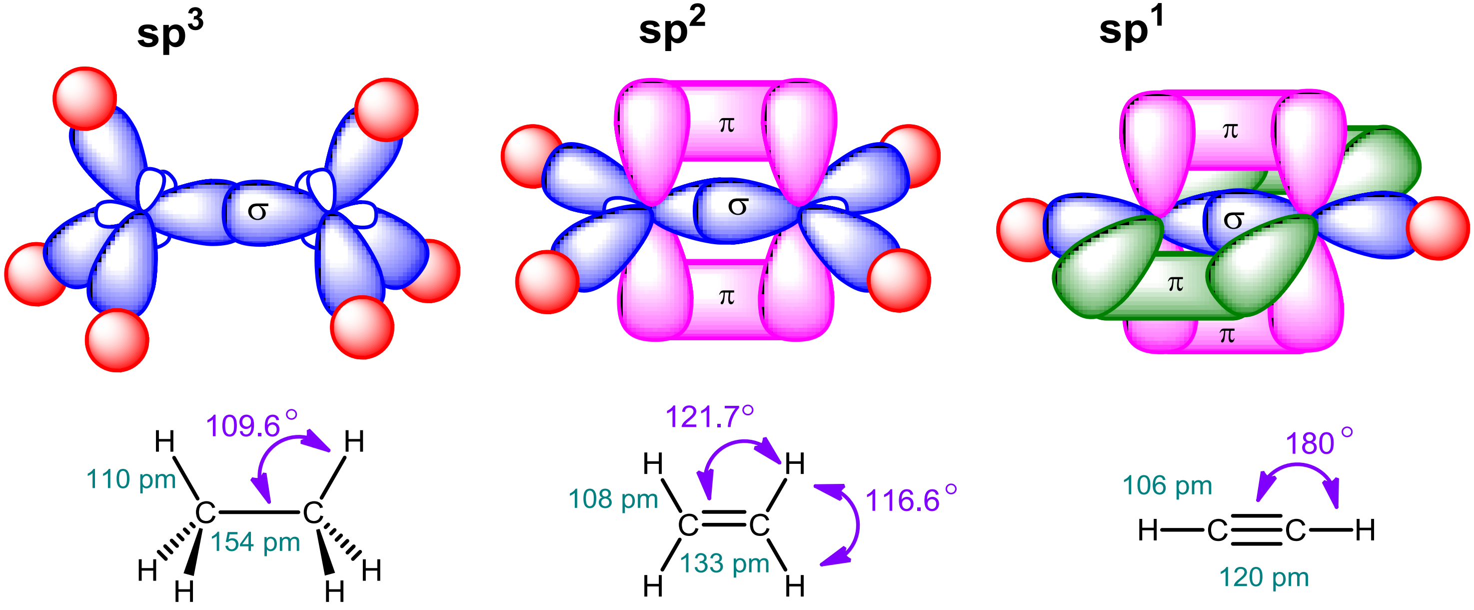




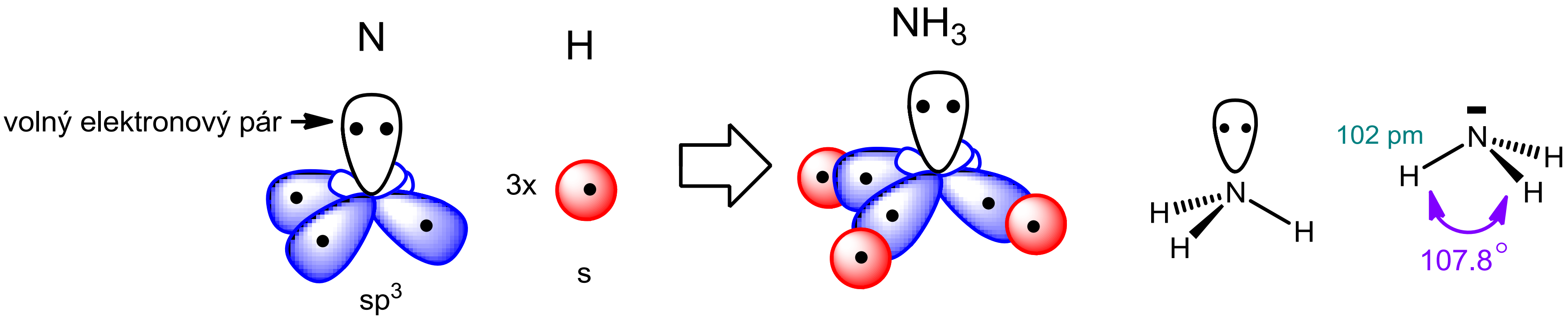
Molekulové orbitaly – trojná vazba C≡C, molekula ethynu

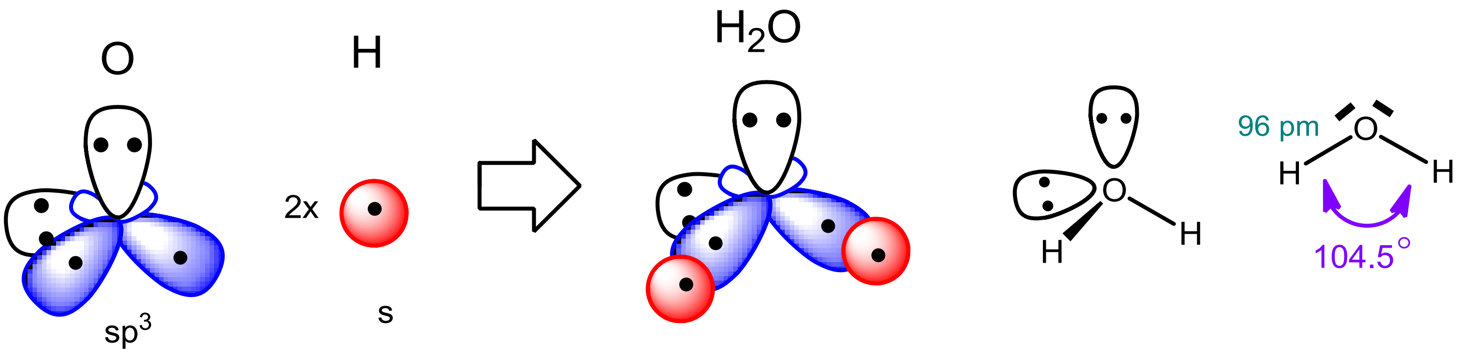




sp3
σ
109.6 °
110 pm
154 pm
H
C
sp2
π
σ
π
121.7°
116.6 °
108 pm
133 pm
sp1
π
σ
π
π
180 °
106 pm
H—C≡C—H
120 pm

Molekulové orbitaly – hybridizace N a O

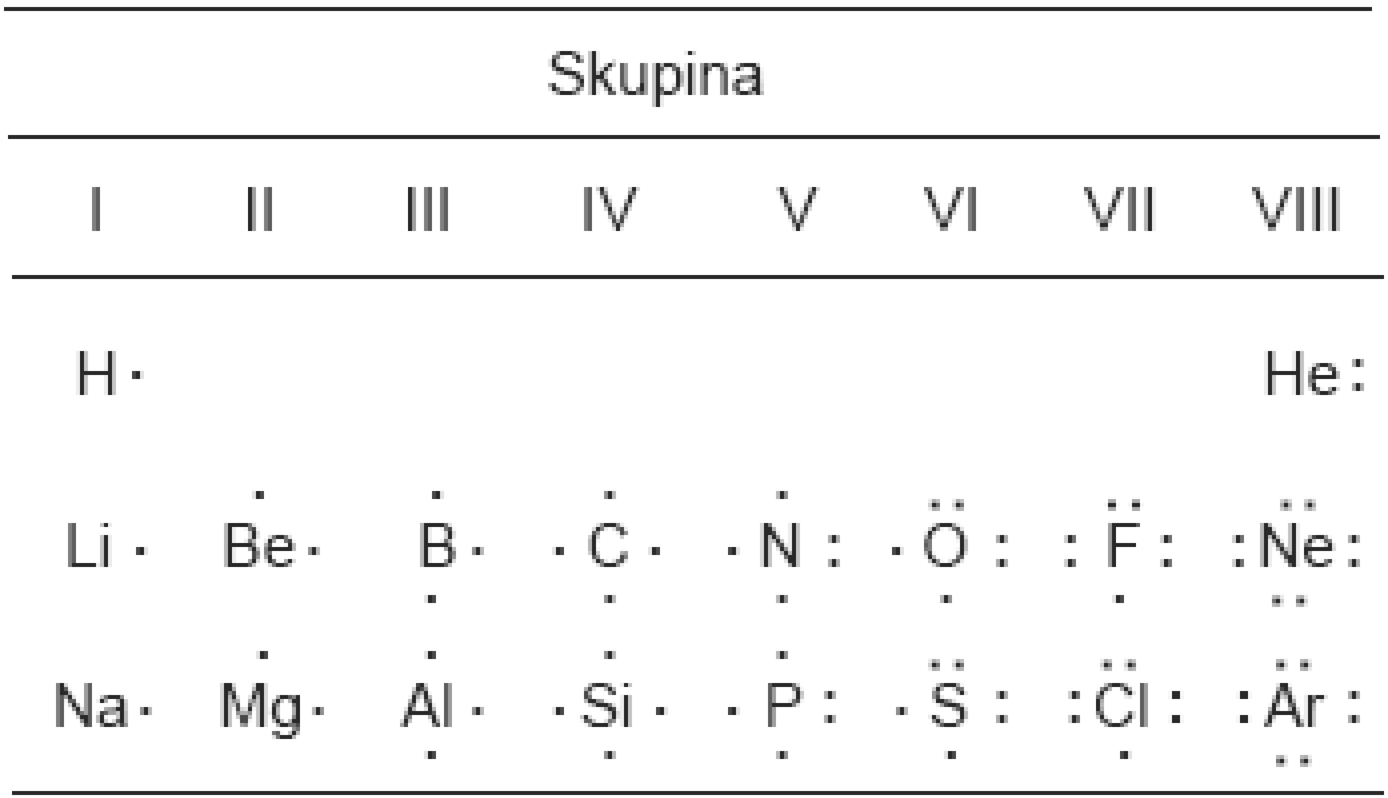




Tabulka 1.2. Elektronové konfigurace prvních 18 prvků.

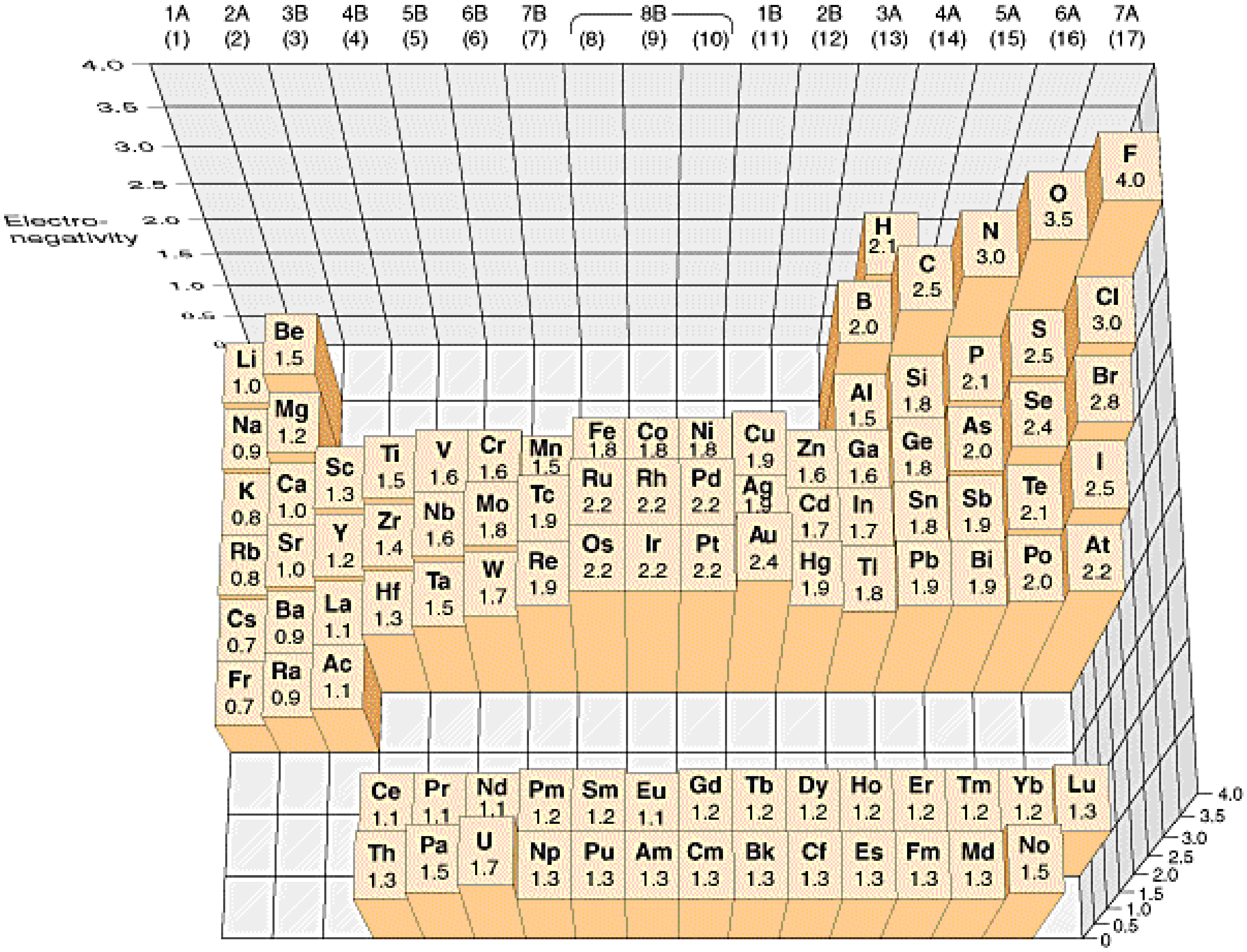
Atomové číslo	Prvek	Počet elektronu v každém orbitalu 1s	2s	2p	3s	3p	Konfigurace
1	H	1					$1s^1$
2	He	2					$1s^2$
3	Li	2	1				$1s^2 2s^1$
4	Be	2	2				$1s^2 2s^2$
5	B	2	2	1			$1s^2 2s^2 2p^1$
6	C	2	2	2			$1s^2 2s^2 2p^2$
7	N	2	2	3			$1s^2 2s^2 2p^3$
8	O	2	2	4			$1s^2 2s^2 2p^4$
9	F	2	2	5			$1s^2 2s^2 2p^5$
10	Ne	2	2	6			$1s^2 2s^2 2p^6$
11	Na	2	2	6	1		$1s^2 2s^2 2p^6 3s^1$
12	Mg	2	2	6	2		$1s^2 2s^2 2p^6 3s^2$
13	Al	2	2	6	2	1	$1s^2 2s^2 2p^6 3s^2 3p^1$
14	Si	2	2	6	2	2	$1s^2 2s^2 2p^6 3s^2 3p^2$
15	P	2	2	6	2	3	$1s^2 2s^2 2p^6 3s^2 3p^3$
16	S	2	2	6	2	4	$1s^2 2s^2 2p^6 3s^2 3p^4$
17	Cl	2	2	6	2	5	$1s^2 2s^2 2p^6 3s^2 3p^5$
18	Ar	2	2	6	2	6	$1s^2 2s^2 2p^6 3s^2 3p^6$

Tabulka 1.3. Valenční elektrony prvních 18 prvků



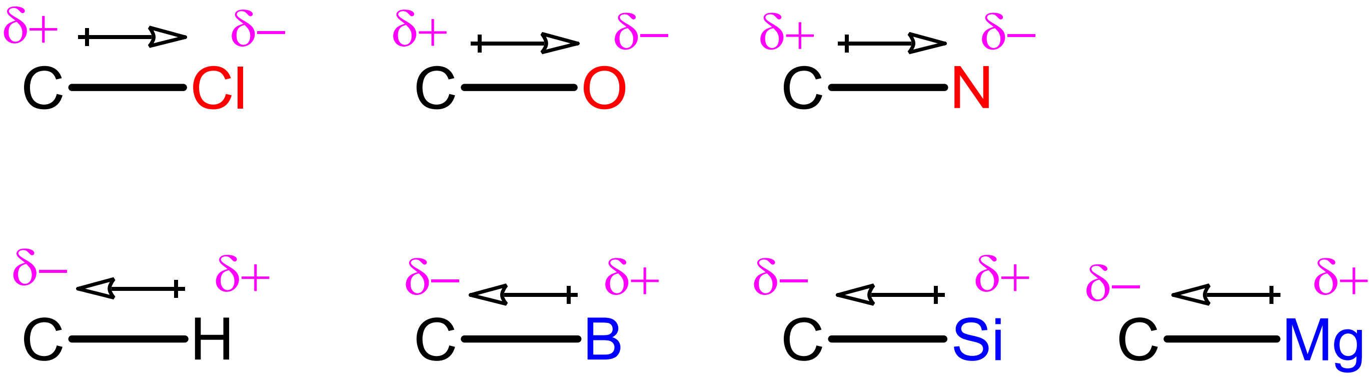
Skupina							
I	II	III	IV	V	VI	VII	VIII
$\mathrm{H}\cdot$							$\mathrm{He}:$
$\mathrm{Li}\cdot$	$\overset{\cdot}{\mathrm{Be}}\cdot$	$\overset{\cdot}{\underset{\cdot}{\mathrm{B}}}\cdot$	$\cdot\overset{\cdot}{\underset{\cdot}{\mathrm{C}}}\cdot$	$\cdot\overset{\cdot}{\underset{\cdot}{\mathrm{N}}}:$	$\cdot\overset{\cdot\cdot}{\underset{\cdot}{\mathrm{O}}}:$	$:\overset{\cdot\cdot}{\underset{\cdot}{\mathrm{F}}}:$	$:\overset{\cdot\cdot}{\underset{\cdot\cdot}{\mathrm{Ne}}}:$
$\mathrm{Na}\cdot$	$\overset{\cdot}{\mathrm{Mg}}\cdot$	$\overset{\cdot}{\underset{\cdot}{\mathrm{Al}}}\cdot$	$\cdot\overset{\cdot}{\underset{\cdot}{\mathrm{Si}}}\cdot$	$\cdot\overset{\cdot}{\underset{\cdot}{\mathrm{P}}}:$	$\cdot\overset{\cdot\cdot}{\underset{\cdot}{\mathrm{S}}}:$	$:\overset{\cdot\cdot}{\underset{\cdot}{\mathrm{Cl}}}:$	$:\overset{\cdot\cdot}{\underset{\cdot\cdot}{\mathrm{Ar}}}:$

Elektronegativita prvků



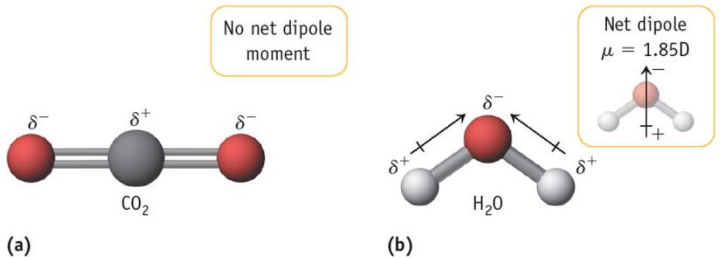
Polarita vazby, induktivní efekt

U kovalentní vazby mezi rozdílnými atomy, nebude elektronový pár oběma atomy sdílen stejně. Jeden atom bude přitahovat elektrony více a jeden méně, dojde k tvorbě tzv. **parciálního náboje** na jednotlivých atomech.
Vzniká **polární kovalentní vazba**.



Posun valenčních elektronů označujeme u polárních kovalentních vazeb jako **induktivní efekt**.
Atomy nebo funkční skupiny, které přitahují elektrony silněji než vodík vykazují ***-I efekt***.
Atomy nebo funkční skupiny, které přitahují elektrony slaběji než vodík vykazují ***+I efekt***.

Dipólový moment



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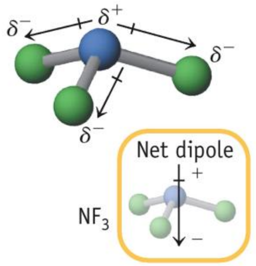

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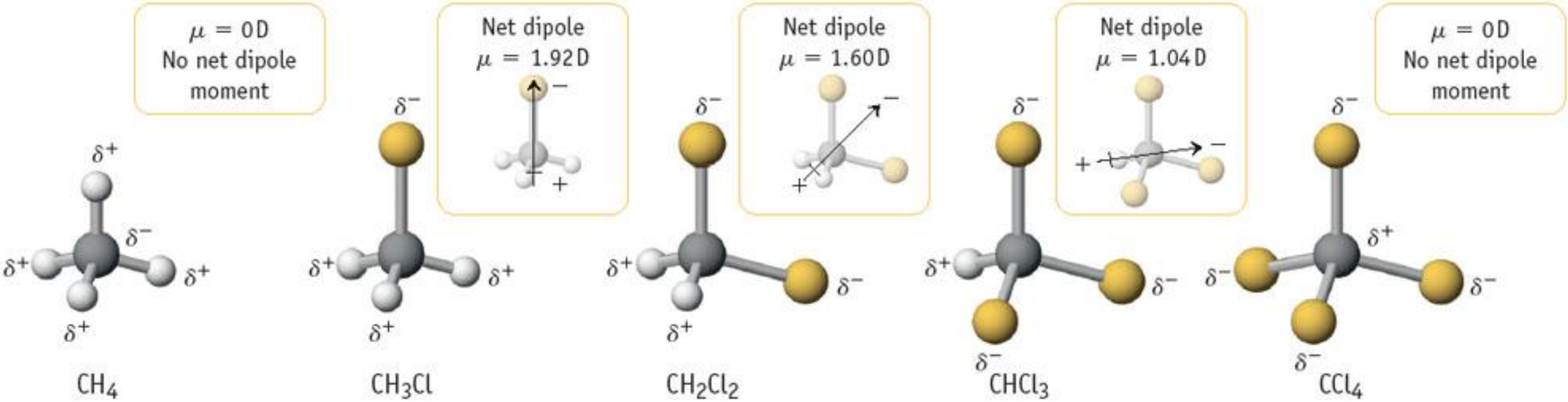

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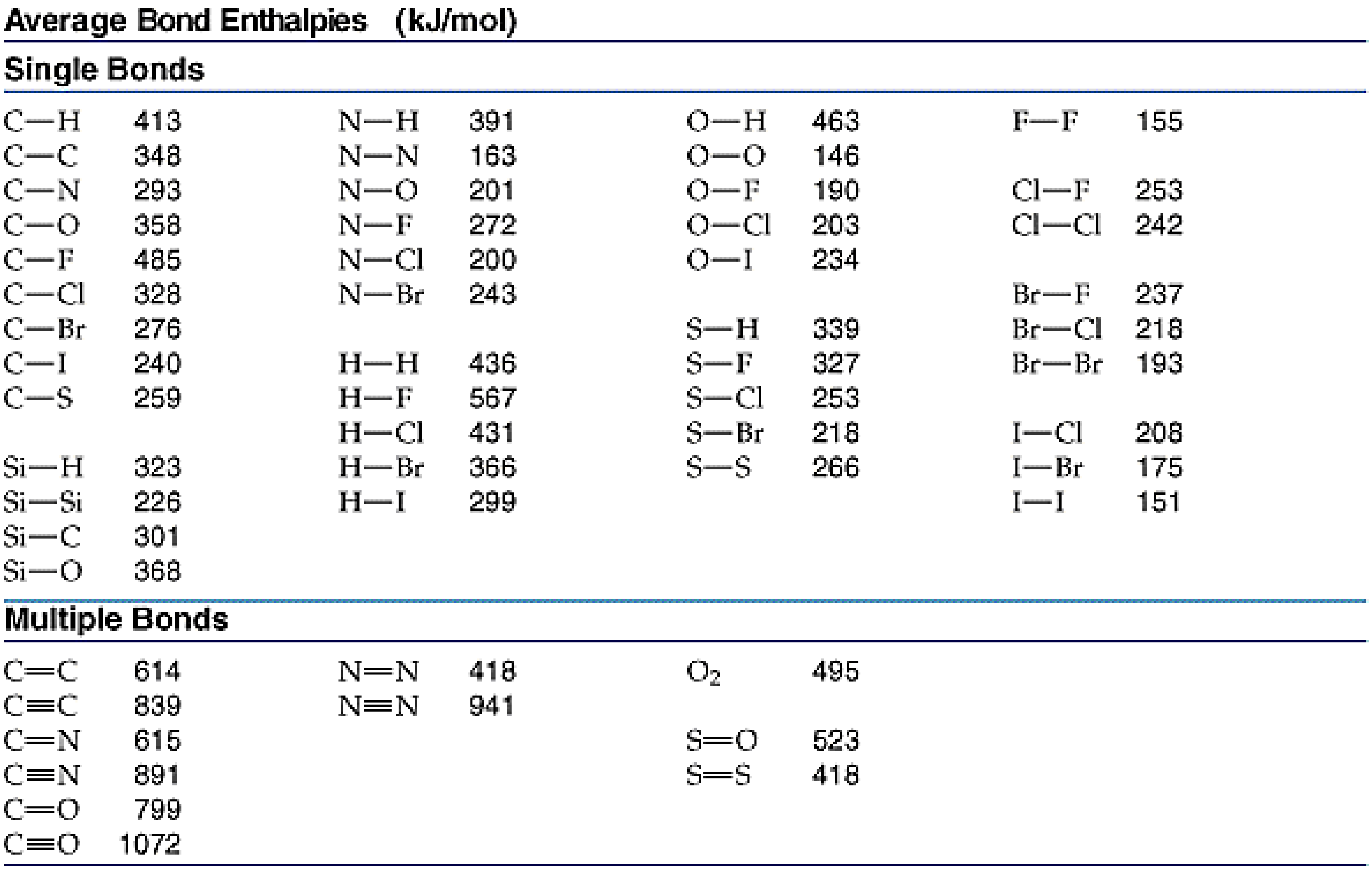
Disociační energie vazeb



Average Bond Enthalpies (kJ/mol)

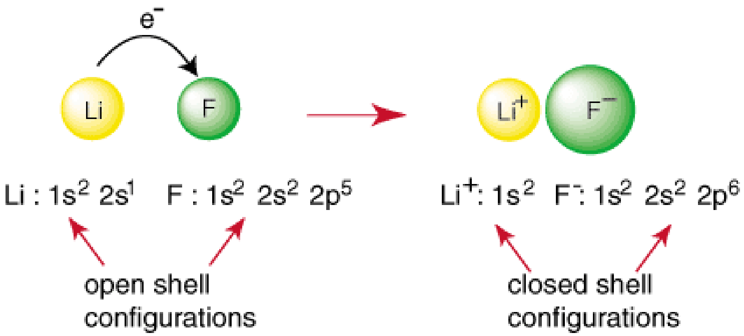
Single Bonds

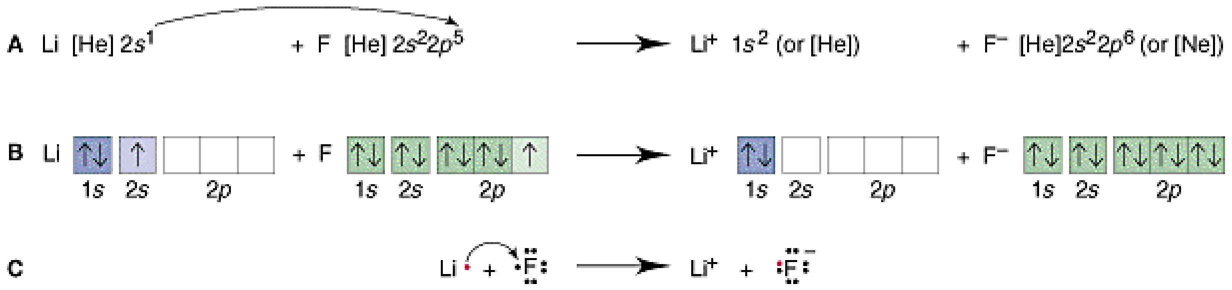
C—H	413	N—H	391	O—H	463	F—F	155
C—C	348	N—N	163	O—O	146		
C—N	293	N—O	201	O—F	190	Cl—F	253
C—O	358	N—F	272	O—Cl	203	Cl—Cl	242
C—F	485	N—Cl	200	O—I	234		
C—Cl	328	N—Br	243			Br—F	237
C—Br	276			S—H	339	Br—Cl	218
C—I	240	H—H	436	S—F	327	Br—Br	193
C—S	259	H—F	567	S—Cl	253		
		H—Cl	431	S—Br	218	I—Cl	208
Si—H	323	H—Br	366	S—S	266	I—Br	175
Si—Si	226	H—I	299			I—I	151
Si—C	301						
Si—O	368						

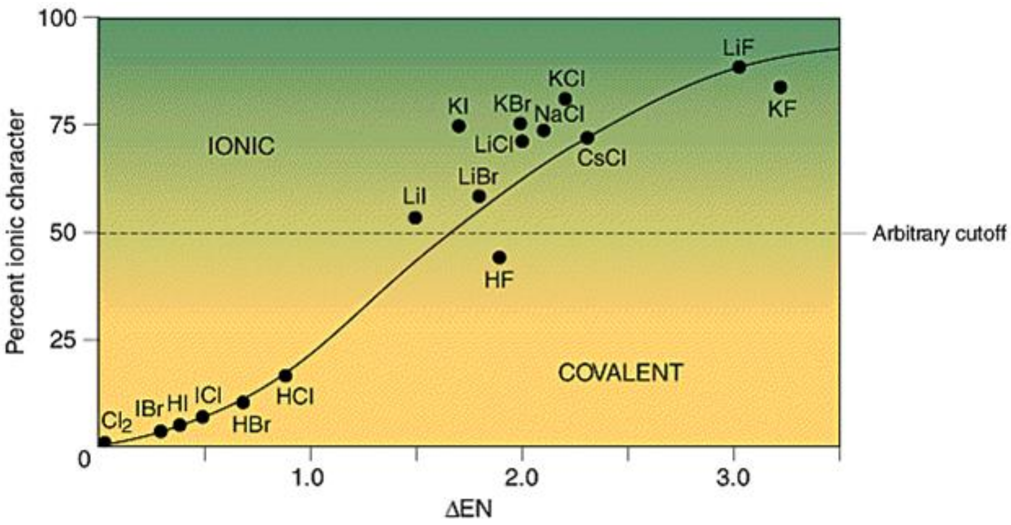
Multiple Bonds

C=C	614	N=N	418	O_2	495
C≡C	839	N≡N	941		
C=N	615			S=O	523
C≡N	891			S=S	418
C=O	799				
C≡O	1072				

Iontová vazba

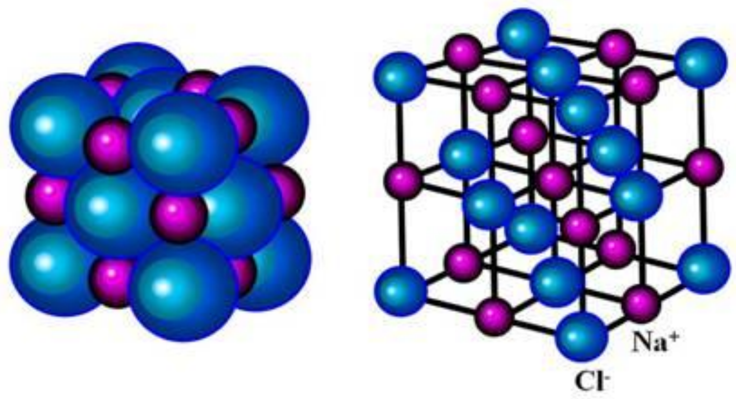




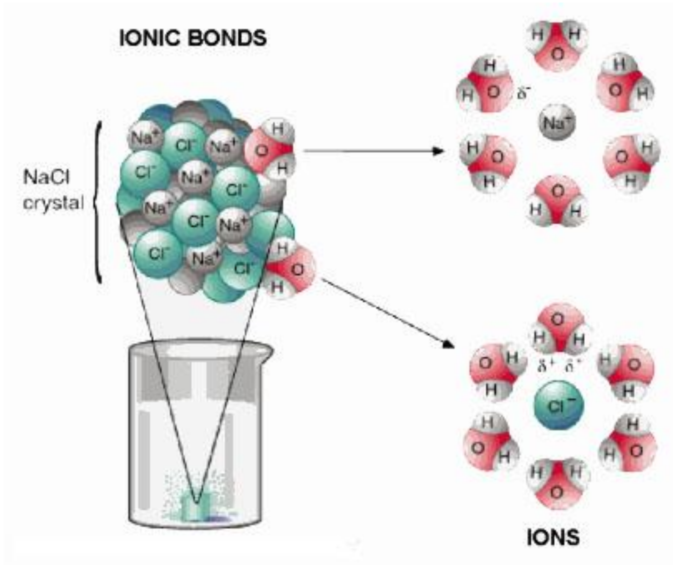


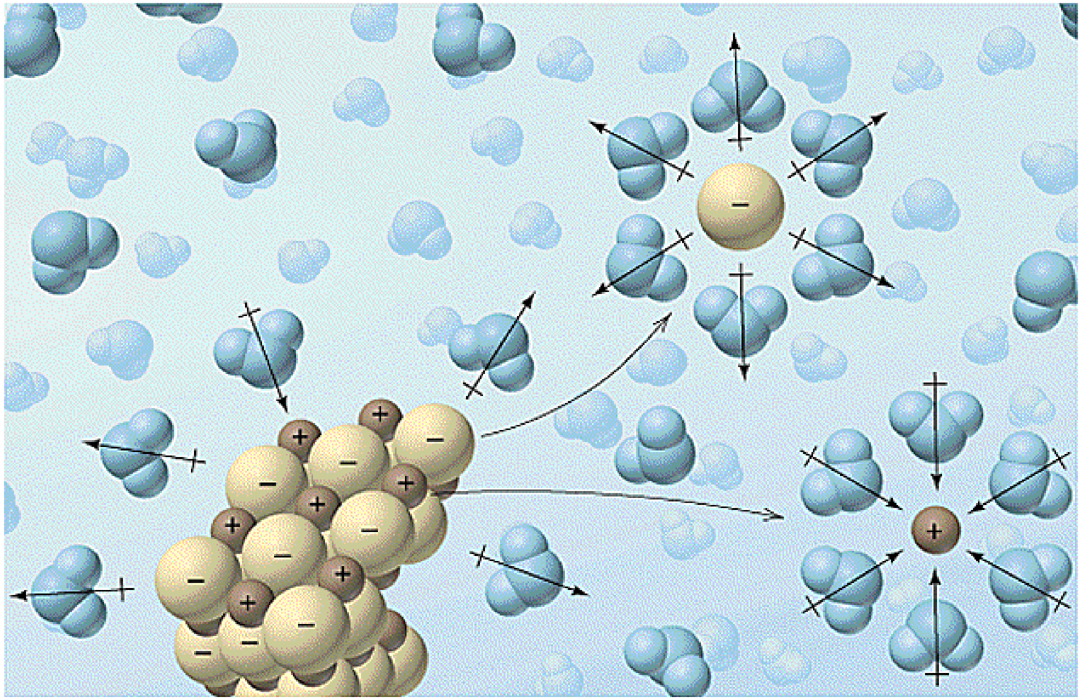
Struktura iontových sloučenin (solí)

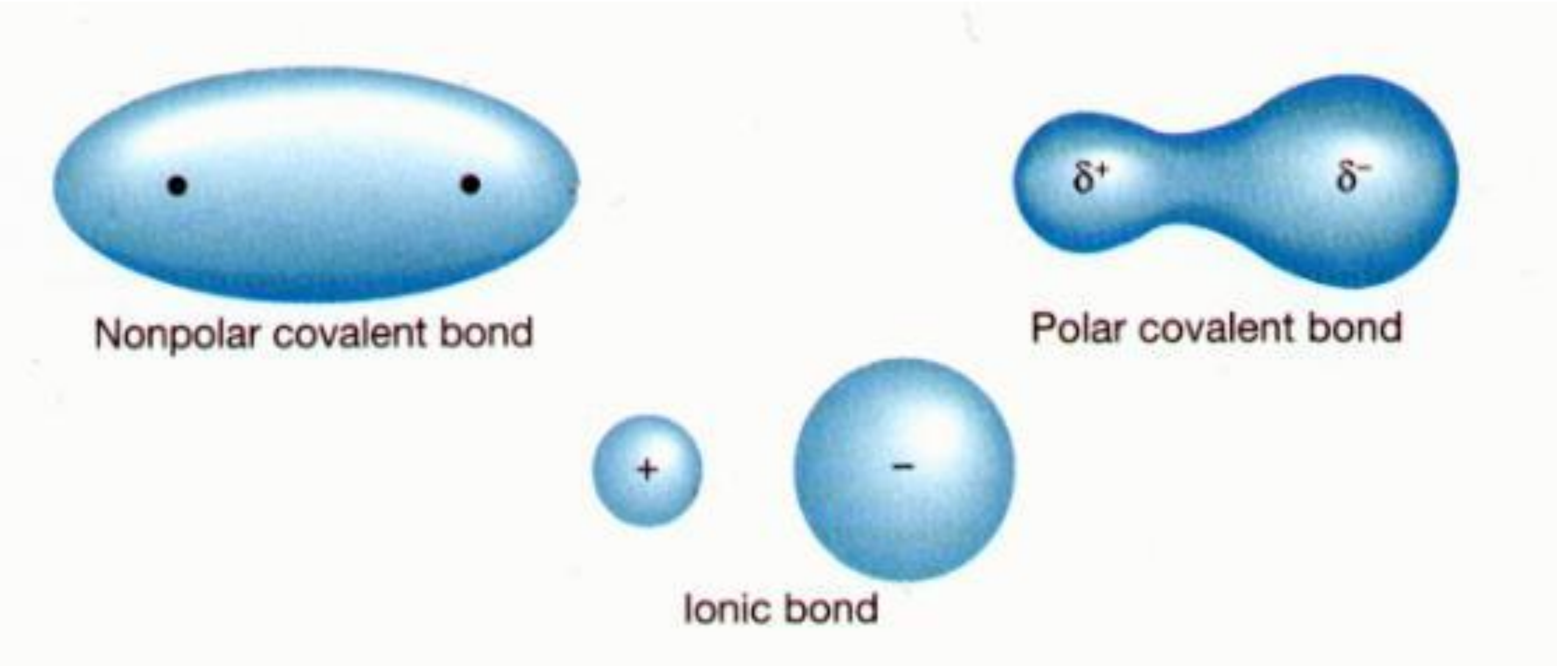
Pevné skupenství – krystalová mřížka



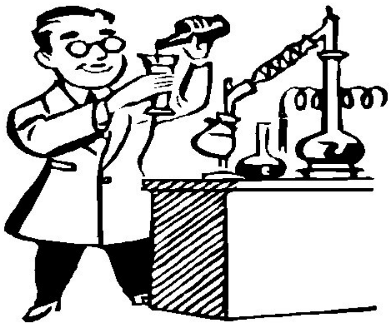
Vodný roztok – solvatace iontů

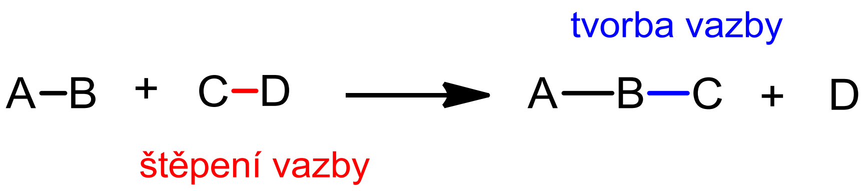





Nonpolar covalent bond
δ+
δ−
Polar covalent bond
+
−
Ionic bond

Chemická reakce – štěpení a tvorba vazeb

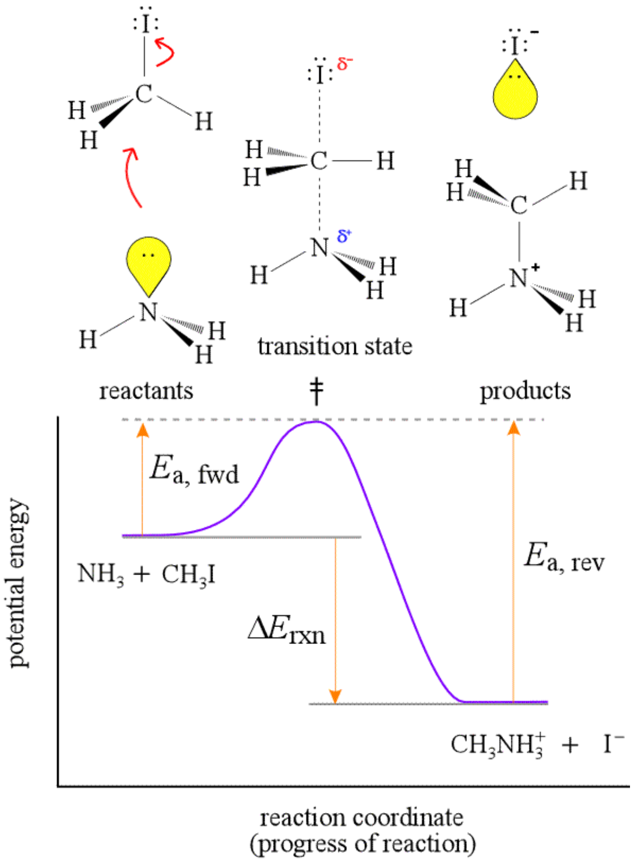


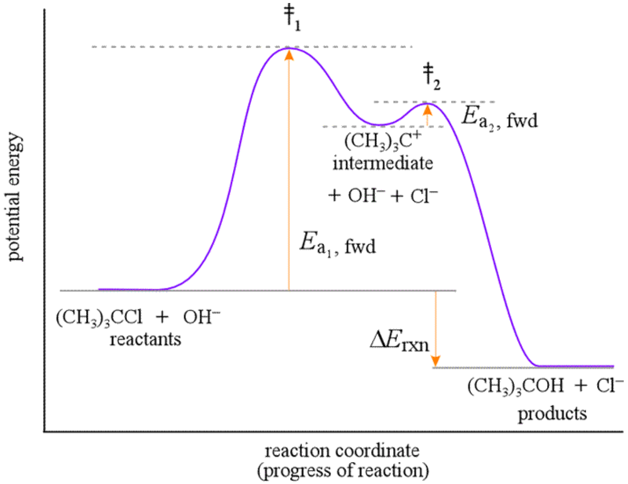


tvorba vazby

$$A-B + C-D \longrightarrow A-B-C + D$$

štěpení vazby



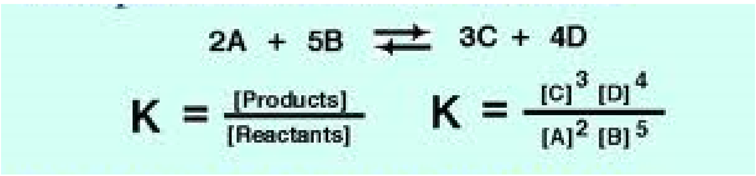


Vratné reakce a reakční termodynamika

vratné reakce

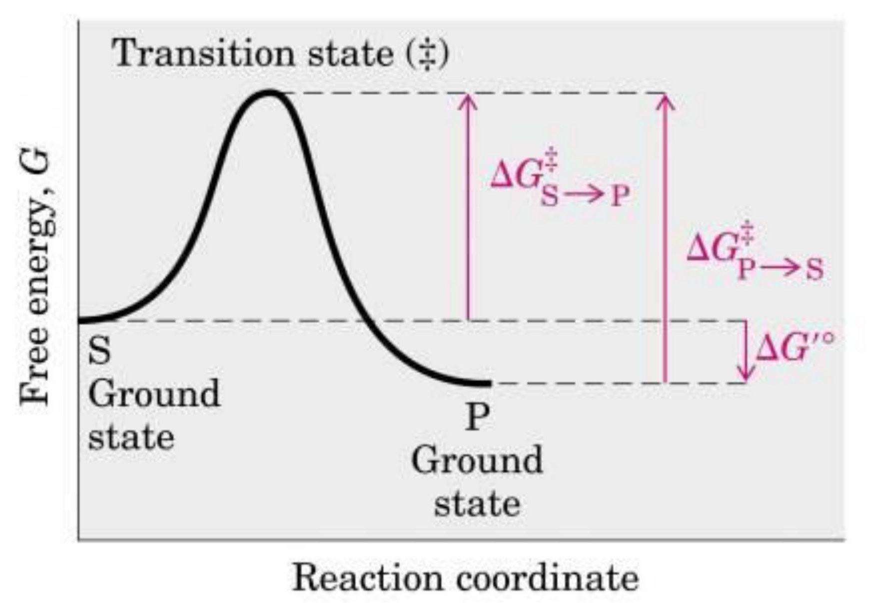
$$A + B \rightleftharpoons C + D$$

Rovnovážná konstanta



$$2A + 5B \rightleftharpoons 3C + 4D$$

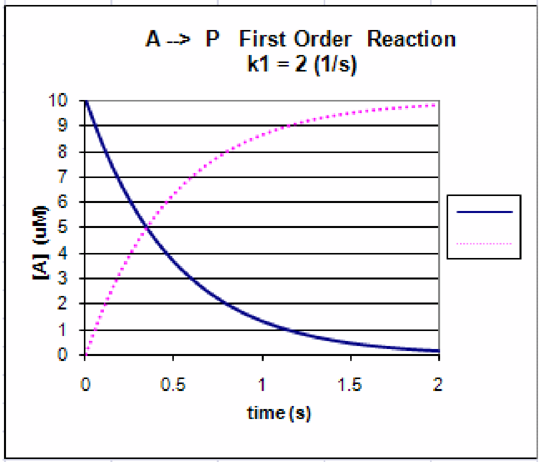
$$K = \frac{[\text{Products}]}{[\text{Reactants}]} \qquad K = \frac{[C]^3\,[D]^4}{[A]^2\,[B]^5}$$



Exotermní reakce – ΔG < 0
Endotermní reakce – ΔG > 0

Reakční kinetika

$$A \xrightarrow{k_1} P$$



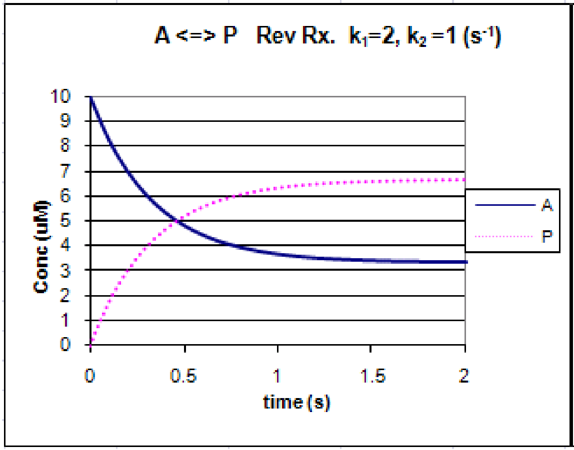
Eyringova rovnice

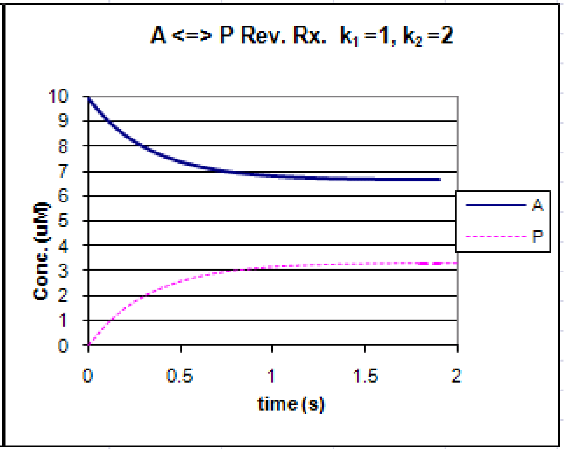
$$k = \frac{k_B T}{h} e^{-\frac{\Delta G^{\ddagger}}{RT}}$$

se zvyšující se teplotou reakční rychlost roste

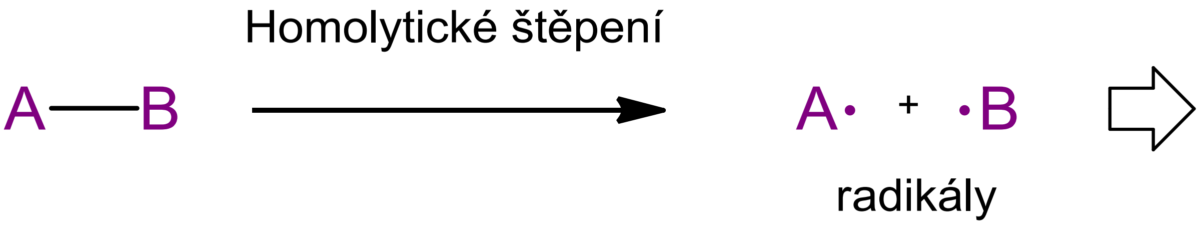
Vratná reakce

$$A \underset{k_2}{\overset{k_1}{\rightleftarrows}} P$$





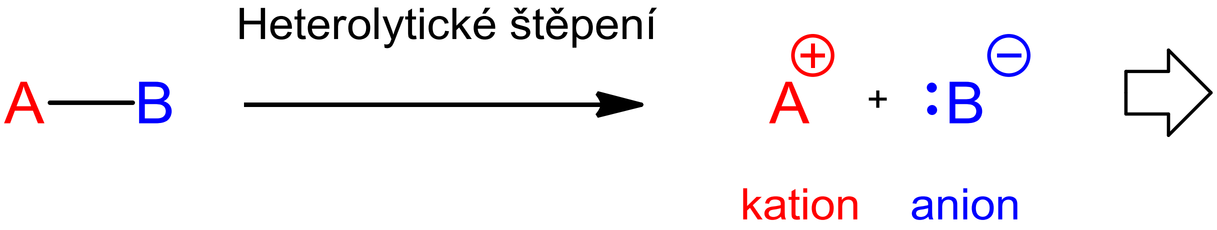
Štěpení vazeb



$$A\text{—}B \xrightarrow{\text{Homolytické štěpení}} A^{\bullet} + {}^{\bullet}B$$

radikály

RADIKÁLOVÉ REAKCE



$$A\text{—}B \xrightarrow{\text{Heterolytické štěpení}} A^{\oplus} + :B^{\ominus}$$

kation anion

POLÁRNÍ REAKCE

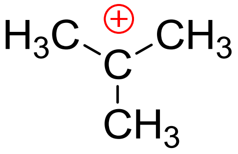
Elektrofilní a nukleofilní reagenty

Polární reakce

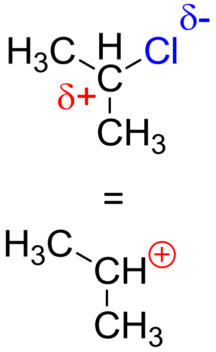
$$\underset{\text{elektrofil}}{E^+} + \underset{\text{nukleofil}}{Nu^-} \longrightarrow E\text{-}Nu$$

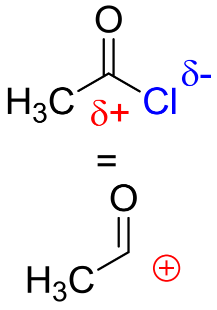
Elektrofilní reagent:

- má afinitu k záporně nabitým částicím
- Jde o kation nebo elektronově chudou neutrální molekulu



$NO_2^{\oplus}$



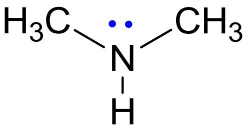


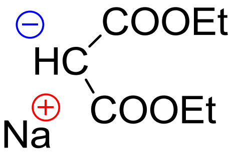
Nukleofilní reagent:

- má afinitu ke kladně nabitým částicím
- Jde o anion nebo elektronově bohatou neutrální molekulu

$OH^{\ominus}$ $OCH_3^{\ominus}$

$:NH_3$





$CH_3\text{-}Li$

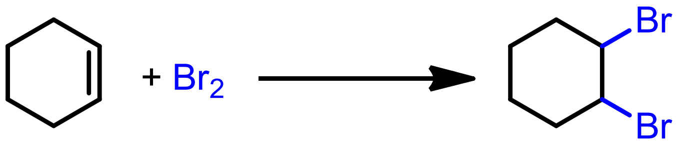
=

$CH_3^{\ominus}$

Typy reakcí v organické chemii

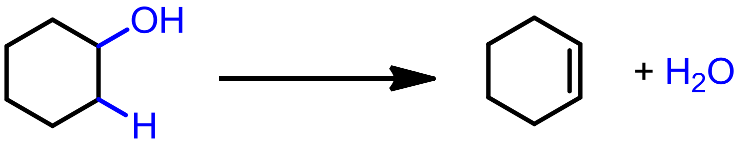
ADICE

A + B → C



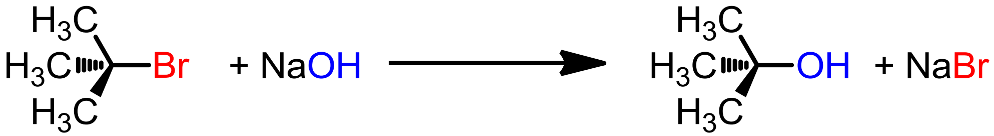
ELIMINACE

A → B + C



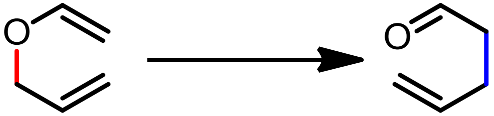
SUBSTITUCE

A-B + C-D → A-D + C-B

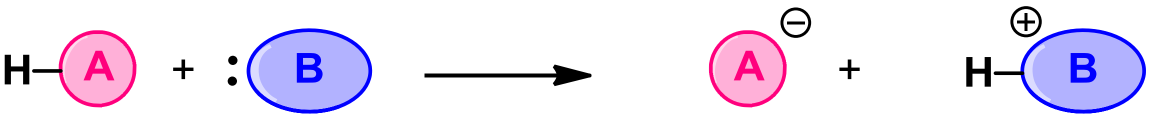


PŘESMYKY

A → B



Kyseliny a báze - Brønstedovy



kyselina **báze** **konjugovaná báze** **konjugovaná kyselina**

$$HCl + NaOH \longrightarrow NaCl + HOH$$

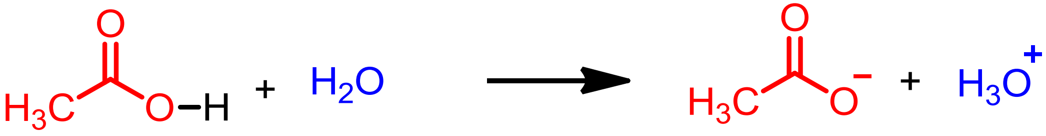
silná kyselina silná báze sůl

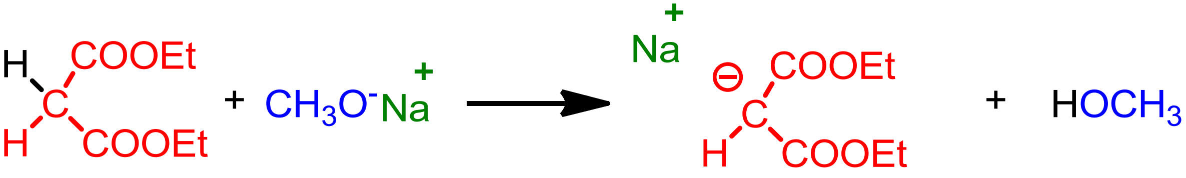
$$HCl + H_2O \longrightarrow Cl^- + H_3O^+$$

silná kyselina slabá báze

$$H_2O + NH_3 \longrightarrow OH^- + NH_4^+$$

slabá kyselina silná báze





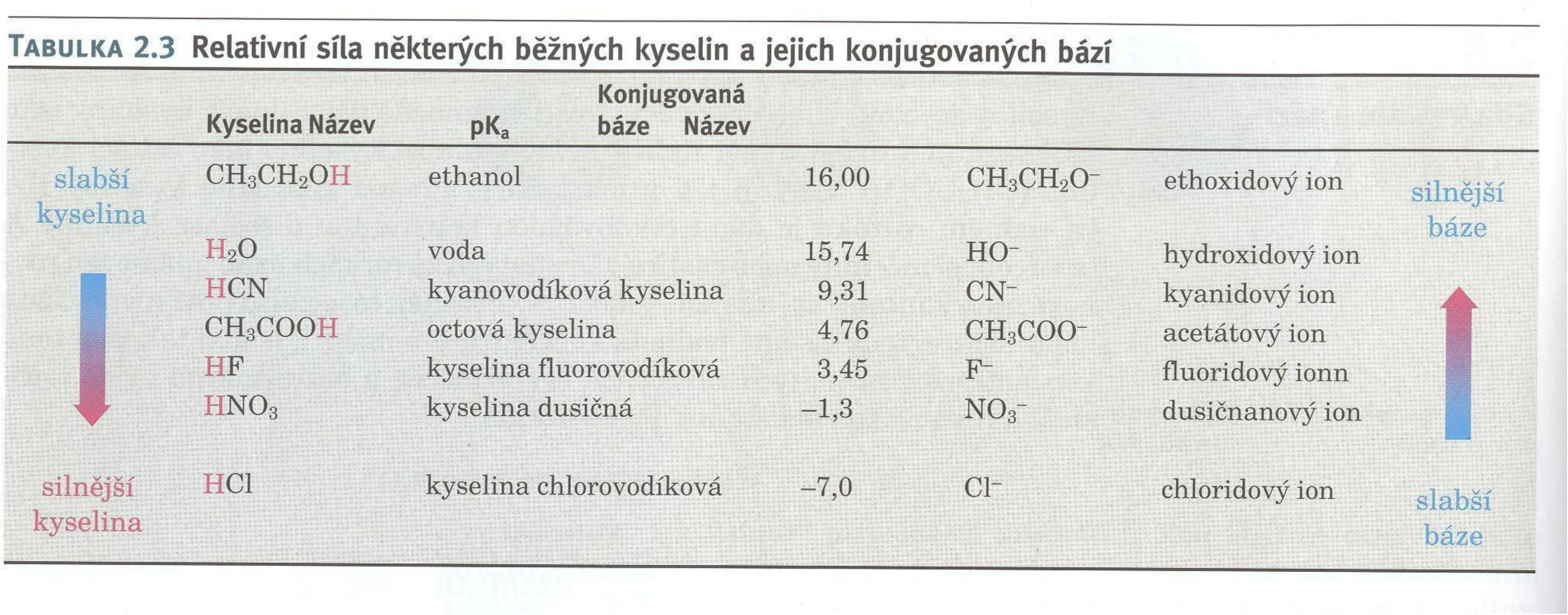
Kyseliny a báze - Brønstedovy

$$HA + H_2O \rightleftharpoons A^- + H_3O^+$$

Rovnovážná konstanta $K = \dfrac{[H_3O^+]\,[A^-]}{[HA]\;[H_2O]}$

Konstanta kyselosti $K_a = K\,[H_2O] = \dfrac{[H_3O^+]\,[A^-]}{[HA]}$

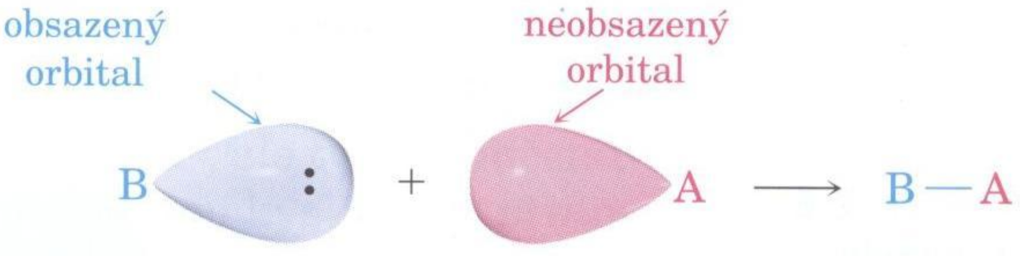
Síla kyseliny se uvává v $pK_a = -\log K_a$



TABULKA 2.3 Relativní síla některých běžných kyselin a jejich konjugovaných bází

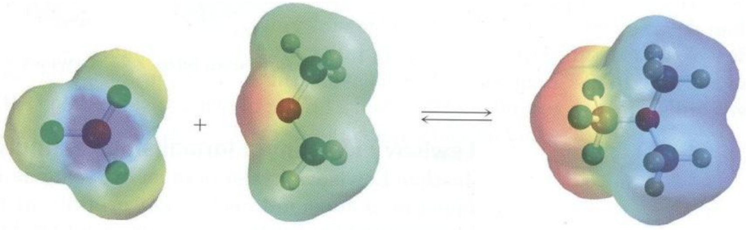
	Kyselina	Název	pK_a	Konjugovaná báze	Název	
slabší kyselina	CH_3CH_2OH	ethanol	16,00	$CH_3CH_2O^-$	ethoxidový ion	silnější báze
	H_2O	voda	15,74	HO^-	hydroxidový ion	
	HCN	kyanovodíková kyselina	9,31	CN^-	kyanidový ion	
	CH_3COOH	octová kyselina	4,76	CH_3COO^-	acetátový ion	
	HF	kyselina fluorovodíková	3,45	F^-	fluoridový ionn	
	HNO_3	kyselina dusičná	–1,3	NO_3^-	dusičnanový ion	
silnější kyselina	HCl	kyselina chlorovodíková	–7,0	Cl^-	chloridový ion	slabší báze

Kyseliny a báze - Lewisovy



Lewisova báze

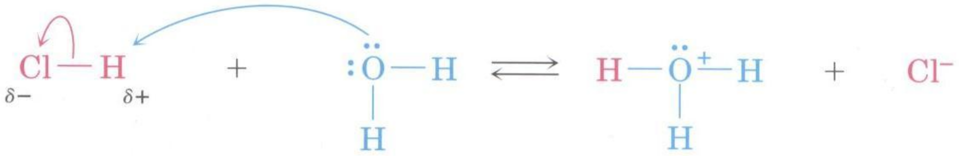
Lewisova kyselina



fluorid boritý

dimethylether

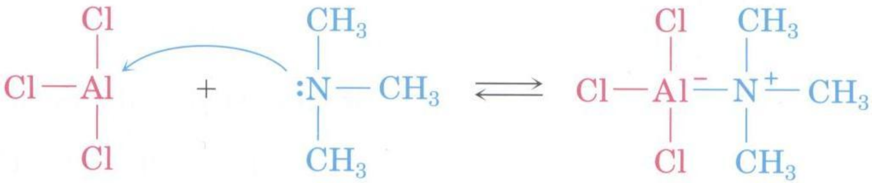
Lewisův acidobazický komplex



chlorovodík (Lewisova kyselina)

voda (Lewisova báze)

oxoniový ion



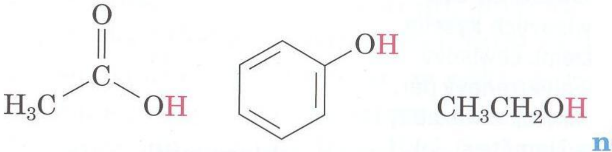
chlorid hlinitý (Lewisova kyselina)

trimethylamin (Lewisova báze)

některé Lewisovy kyseliny

neutrální donory protonů:

H_2O HCl HBr HNO_3 H_2SO_4



karboxylová kyselina **fenol** **alkohol**

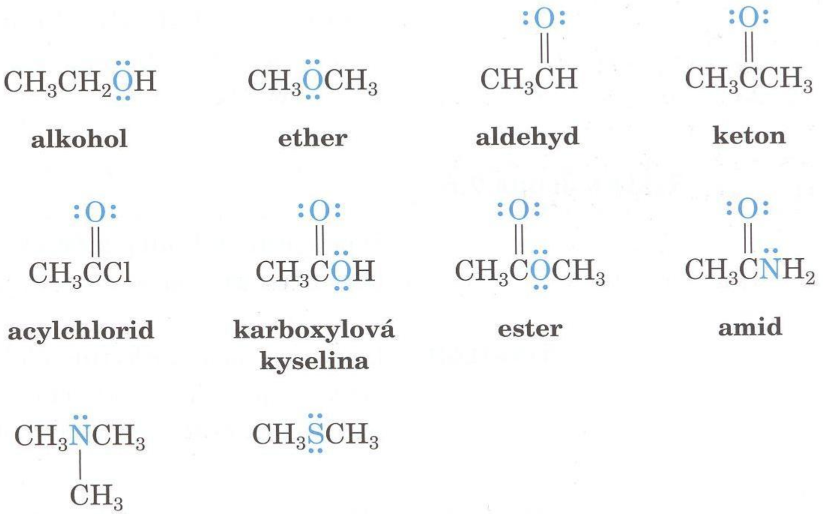
některé kationty:

Li^+ Mg^{2+} Br^+

některé sloučeniny kovů

$AlCl_3$ BF_3 $TiCl_4$ $FeCl_3$ $ZnCl_2$

některé Lewisovy báze


$CH_3CH_2\ddot{O}H$ **alkohol**

$CH_3\ddot{O}CH_3$ **ether**

$CH_3CH{=}\ddot{O}$ **aldehyd**

CH_3CCH_3 ($C{=}\ddot{O}$) **keton**

CH_3CCl ($C{=}\ddot{O}$) **acylchlorid**

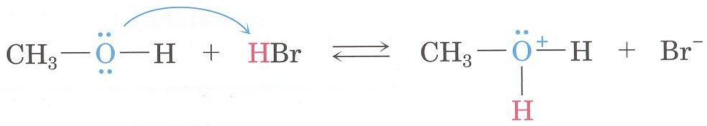
$CH_3C\ddot{O}H$ ($C{=}\ddot{O}$) **karboxylová kyselina**

$CH_3C\ddot{O}CH_3$ ($C{=}\ddot{O}$) **ester**

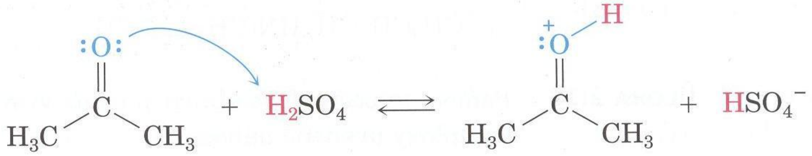
$CH_3C\ddot{N}H_2$ ($C{=}\ddot{O}$) **amid**

$CH_3\ddot{N}CH_3$ ($N{-}CH_3$) **amin**

$CH_3\ddot{S}CH_3$ **sulfid**

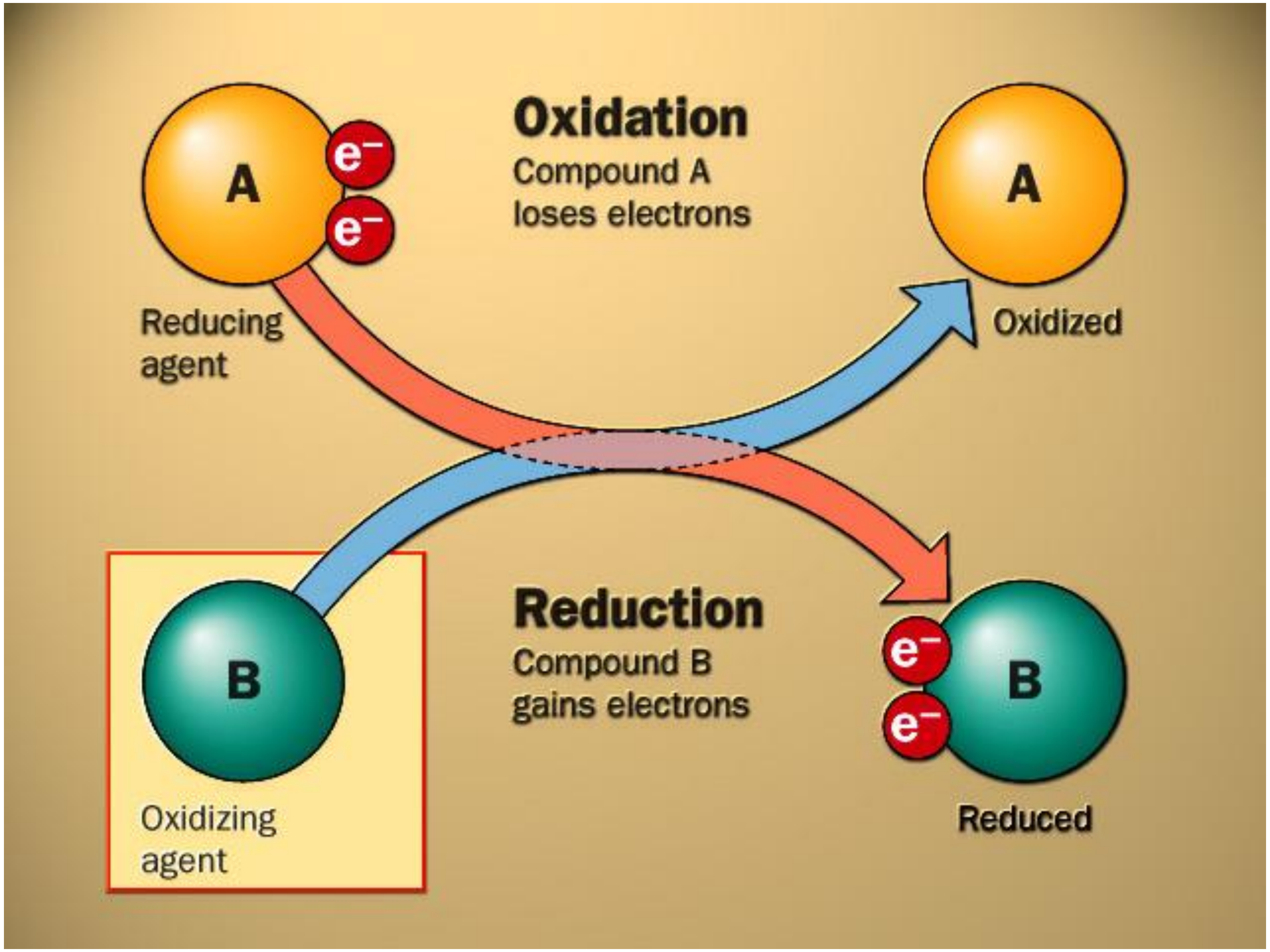


methanol **(báze)** **bromovodík** **(kyselina)** **methyloxonium-bromid**



aceton **(báze)** **kyselina sírová**

Redoxní reakce – oxidace a redukce



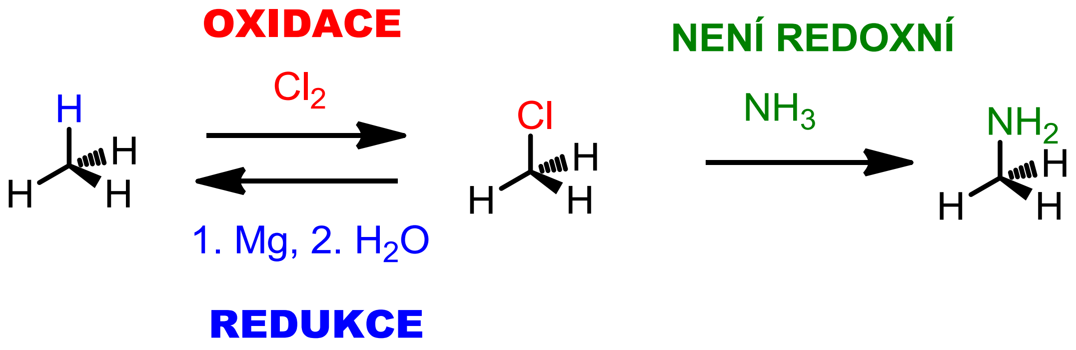
Redoxní reakce – oxidace a redukce

Oxidace – dochází ke **snížení elektronové hustoty na atomu uhlíku**

- tvorbou vazeb C-O, C-N, C-X nebo C=C
- zánikem vazeb C-H

Redukce – dochází ke **zvýšení elektronové hustoty na atomu uhlíku**

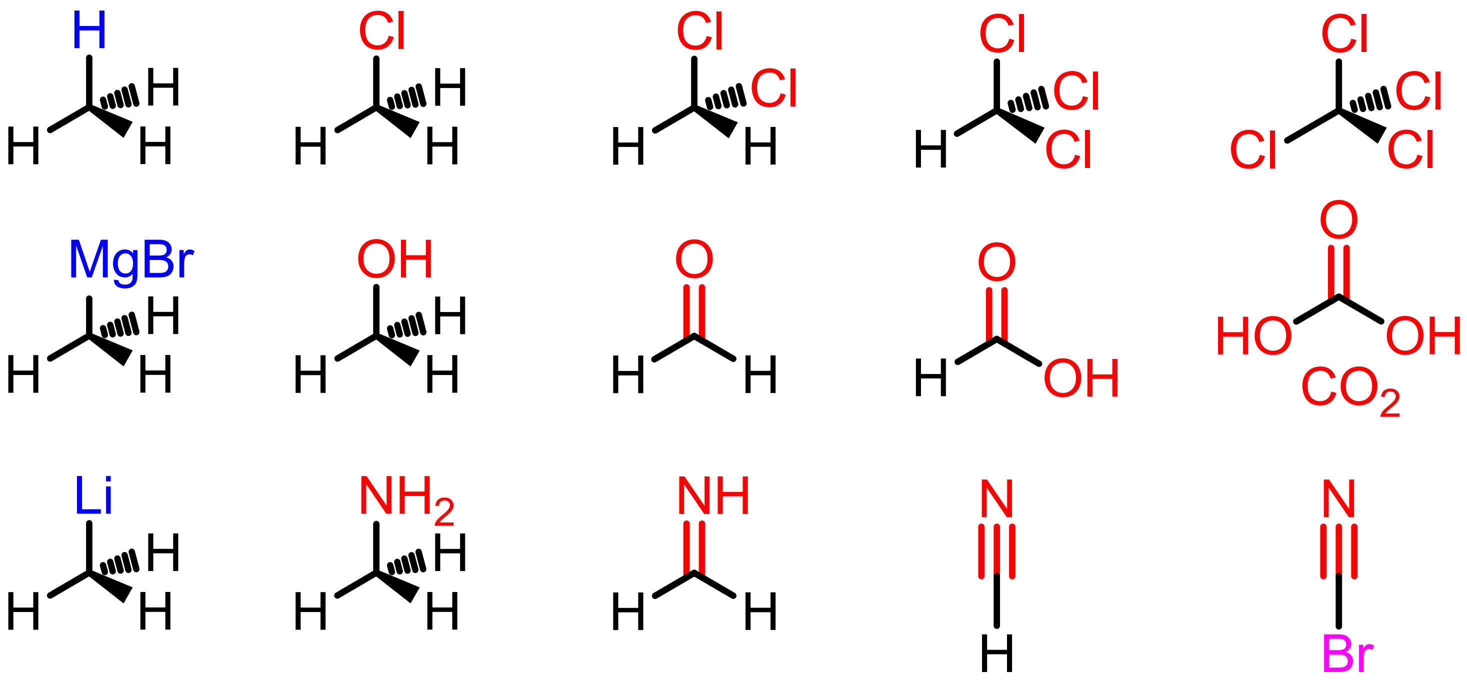
- zánikem vazeb C-O, C-N, C-X nebo C=C
- tvorbou vazeb C-H nebo C-kov



Redoxní reakce – oxidační stupeň

Deriváty methanu

-IV **-II** **0** **+II** **+IV**



Redoxní reakce – oxidace a redukce

Deriváty vyšších uhlovodíků (R = alkyl)

-V **-III** **-I** **+I**