

Bonding in organic molecules

Dissociation energies of some bonds [kJ/mol]

C-H	413	C-C	346	C=C	610	C≡C	837
C-N	309	C=N	615	C≡N	887	C-S	272
C-Cl	339	C-Br	284	C-I	213	N-N	163
O-O	166	O=O	498	S-S	226	F-F	153
I-I	151	H-O	463	H-N	391	H-S	347
H-Br	366	H-I	299	O-Cl	217	O-Br	201
C-O	357	C=O	737	C=S	535	C-F	444
N=N	418	N≡N	941	Br-Br	193	Cl-Cl	243
H-F	570	H-Cl	431				

Dissociation energies of C-H bonds in connection with the structure of hydrocarbon skeleton [kJ/mol]

CH ₃ -H	427	$\begin{array}{l} \text{CH}_3 \\ \diagdown \\ \text{CH-H} \\ \diagup \\ \text{CH}_3 \end{array}$	393	C ₆ H ₅ -H	427
C ₂ H ₅ -H	405			C ₆ H ₅ -CH ₂ -H	326
n-C ₃ H ₇ -H	405	(CH ₃) ₃ C-H	381	CH ₂ =CH-H	435

Bonding in organic molecules

Average bond length in organic molecules [nm]

C-C	0,154	C=C	0,134	C≡C	0,120
C-H	0,111	C-O	0,141	C=O	0,120
C-N	0,147	C=N	0,128	C≡N	0,116
C-S	0,181	C=S	0,156	C-F	0,138
C-Cl	0,178	C-Br	0,194	C-I	0,214

Bonding in organic molecules

LA CHE MA pharmaceuticals
diagnostica
chimica

PERIODICKÁ SOUSTAVA PRVKŮ

Atomová hmotnost
značka (symbol)
protonové číslo

elektronová konfigurace
Atomová hmotnost

akronogativa
Český název
stříbrný název

FORMULY

I.A		d										II.A	III.A	IV.A	V.A	VI.A	VII.A	VIII.A	
1,008 1 H VODÍK Hydrogenium													4,00 2 He HELIUM Helium						
6,94 3 Li LITHIUM Lithium	9,01 4 Be BERYLÍUM Beryllium												10,81 5 B BOR Bor	12,01 6 C UHLÍK Carbonium	14,01 7 N DUSÍK Nitrogenium	16,00 8 O KYSLÍK Oxygenium	19,00 9 F FLUOR Fluorium	20,18 10 Ne NEON Neon	
22,99 11 Na SODÍK Natrium	24,31 12 Mg HOŘÍK Magnesium												26,98 13 Al HLÍZEK Aluminium	28,09 14 Si KŘÍDELO Silicium	30,07 15 P FOSFOR Phosphorus	32,06 16 S SIŘIČKA Sulfur	35,45 17 Cl CHLÓR Chlorium	39,95 18 Ar ARGON Argon	
39,10 19 K DRAŽEK Kalium	40,08 20 Ca VÁPNEK Calcium	44,96 21 Sc SKANDIUM Scandium	47,88 22 Ti TITAN Titanium	50,94 23 V VANAD Vanadium	52,00 24 Cr CHROM Chromium	54,94 25 Mn MANGAN Manganium	58,93 26 Fe ŽELEZO Ferrum	58,93 27 Co KOBALT Cobaltum	58,93 28 Ni NIKEL Nickelium	63,55 29 Cu MĚD Cuprum	65,38 30 Zn ZINEK Zincum	69,72 31 Ga GALIEK Gallium	72,64 32 Ge GERMANIUM Germanium	74,92 33 As ARSEN Arsenicum	78,96 34 Se SELENIUM Selenium	79,90 35 Br BROM Bromium	83,80 36 Kr KRYPTON Krypton		
85,47 37 Rb RUBIDIUM Rubidium	87,62 38 Sr STRONCIUM Strontium	88,91 39 Y YTRIJUM Yttrium	91,22 40 Zr CERIJUM Zirconium	92,91 41 Nb NIOBIUM Niobium	95,94 42 Mo MOLYBDÉN Molybdenum	97,91 43 Tc TECHNETIUM Technetium	101,07 44 Ru RUTHENIUM Ruthenium	101,07 45 Rh RHODIUM Rhodium	101,07 46 Pd PALADIUM Palladium	106,37 47 Ag STŘEBRO Argentum	107,87 48 Cd KADMIUM Cadmium	112,41 49 In INDIUM Indium	118,71 50 Sn CIN Stannum	121,76 51 Sb ANTIMON Antimonium	127,60 52 Te TELUR Tellurium	126,91 53 I JOD Iodum	131,30 54 Xe KSIEN Xenon		
132,91 55 Cs CEZIJUM Caesium	137,33 56 Ba BARIUM Barium	138,91 57 La LANTHAN Lanthanum	178,49 72 Hf HAFNIUM Hafnium	180,95 73 Ta TANTAL Tantalum	183,85 74 W WOLFRAM Wolframium	186,21 75 Re RHENIUM Rhenium	186,21 76 Os OSMIUM Osmium	186,21 77 Ir IRIDIUM Iridium	186,21 78 Pt PLATINA Platinum	196,97 79 Au ZLATO Aurum	200,59 80 Hg RTUŤ Hydrargyrum	204,39 81 Tl THALLIUM Thallium	208,98 82 Pb OLOVO Plumbum	208,98 83 Bi BISMUT Bismutum	208,98 84 Po POLONIUM Polonium	208,98 85 At ASTAT Astatium	222 86 Rn RADON Radon		
223,02 87 Fr FRANCIUM Francium	226,02 88 Ra RADIUM Radium	227,03 89 Ac AKTINIUM Actinium	238,03 92 U URAN Uranium	238,03 93 Np NEPTUNIUM Neptunium	238,03 94 Pu PLUTONIUM Plutonium	238,03 95 Am AMERICIUM Americium	238,03 96 Cm CURIUM Curium	238,03 97 Bk BERKELIUM Berkelium	238,03 98 Cf KALIFORNIUM Californium	238,03 99 Es EINSTEINIUM Einsteinium	238,03 100 Fm FERMIUM Fermium	238,03 101 Md MEDELERIUM Mendelevium	238,03 102 No NORBOLIV Nobelium	238,03 103 Lr LAVRENCIUM Lawrencium					

Prvky: zásadotvorné slabé amfoterní kyselinotvorná slabé inertní umělé

Skupenství prvků (př 30°C): He – plyné, Hg – kapalné, Fe – pevné

Bonding in organic molecules

Elements
electronegativity

C	2,55
H	2,20
O	3,44
N	3,04
Cl	3,16
Br	2,96
I	2,66
S	2,58

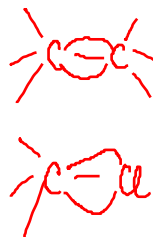
DIPOLE MOMENT

$$\mu = e \cdot d$$

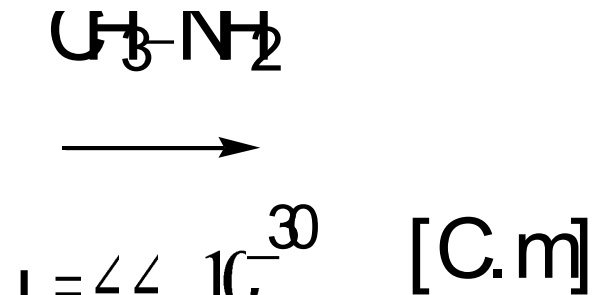
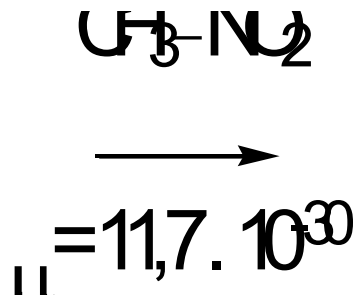
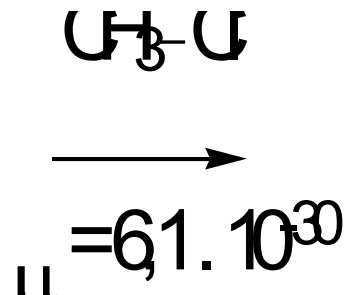
e atom charge [C]

d distance [m]

Dipole moment is a **vector** – with value and direction

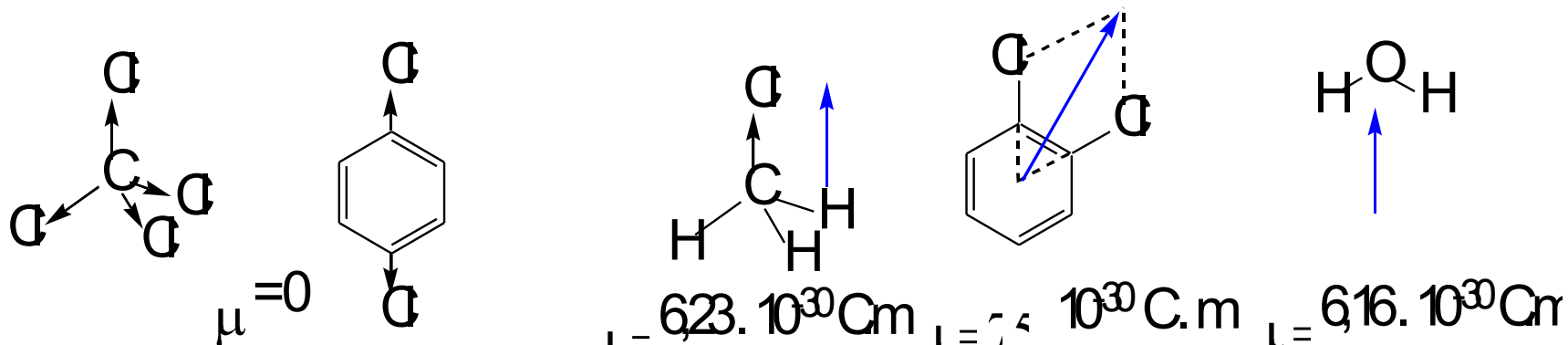


	μ		μ
H - C	1,33	C - N	0,73
H - N	4,36	C - O	2,46
H - O	5,03	C = O	7,65
		C \equiv N	11,65



Bonding in organic molecules

Dipole moment - vector



Most of reactions is realized in a solvent , that by the solvation can influence the charge distribution in the molecule

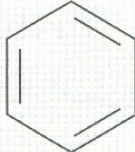
In the older literature you can find expression of dipole moment in units **D**

$$1\text{D} = 3,33564 \cdot 10^{-30} \text{ C} \cdot \text{m}$$

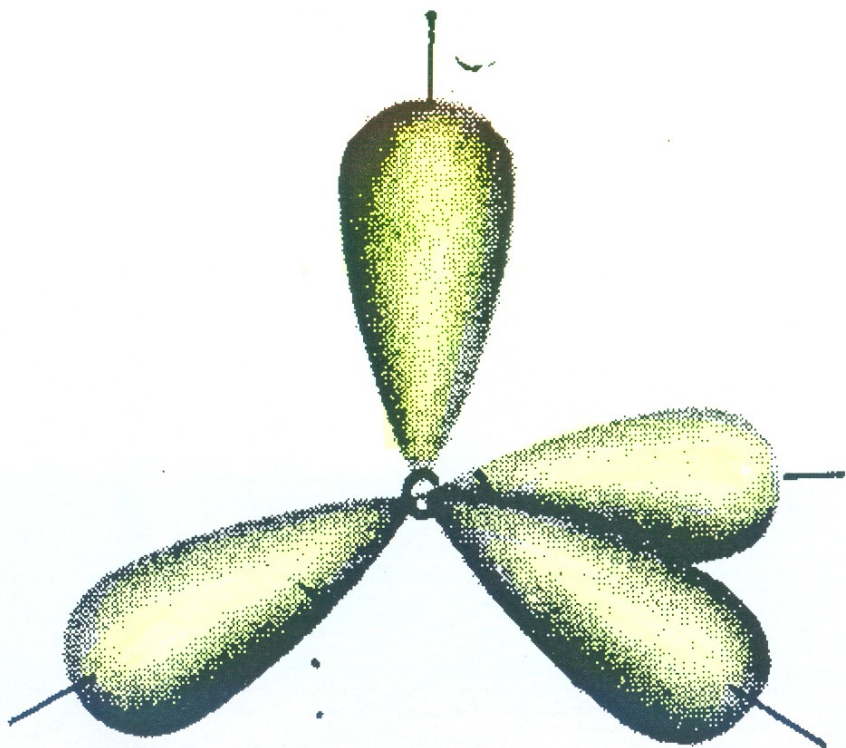
Bonding in organic molecules

Dipole moment - vector

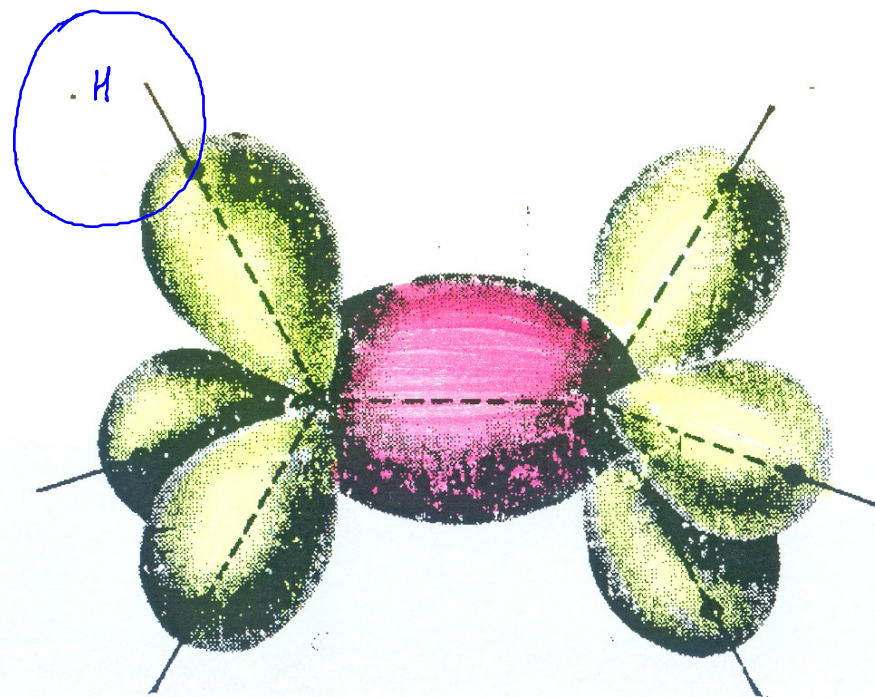
Dipole moments of some molecules

Compound	Dipole moment		Compound	Dipole moment	
	10^{30} C m	D		10^{30} C m	D
NaCl	30,02	9,0	NH ₃	4,90	1,47
$\text{H}_3\text{C}-\overset{\text{+}}{\text{N}}\begin{matrix} \text{=O} \\ \text{O}^- \end{matrix}$ nitromethan	11,54	3,46	CH ₄	0	0
CH ₃ Cl	6,24	1,87	CCl ₄	0	0
H ₂ O	6,17	1,85	CH ₃ CH ₃	0	0
CH ₃ OH	5,67	1,70	 benzen	0	0
$\text{H}_2\text{C}=\overset{\text{+}}{\text{N}}=\text{N}^-$ diazomethan	5,00	1,50	BF ₃	0	0

Bonding in organic molecules



Carbon atom in sp³ state



Bond C-C by overlap of sp³ orbitals

Bonding in organic molecules

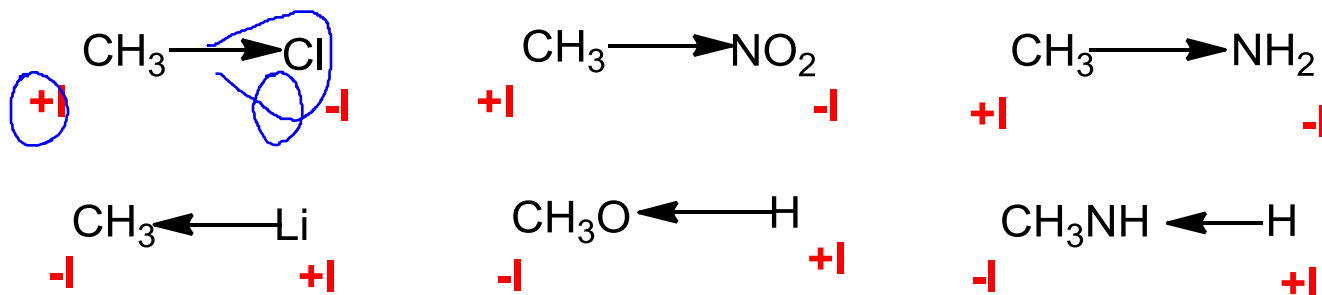
Elektronegativity of elements

C	2,55
H	2,20
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Bond polarity Inductive effekt

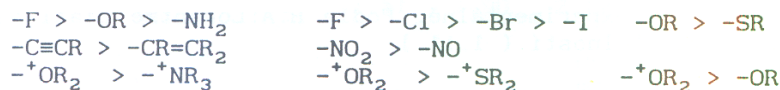
Based upon different electronegativity of bonded atoms, the electrons in bonds are shifted more or less in the bond towards one of the atoms.

The shift in single bonds (σ -bonds) is called **inductive effect**

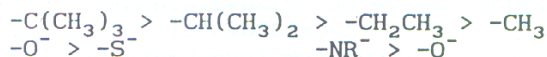


Inductive effects of some atoms and groups

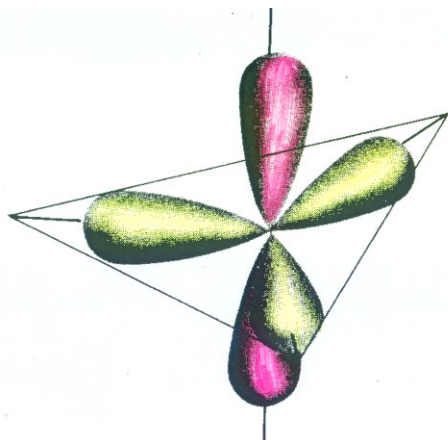
- I effect



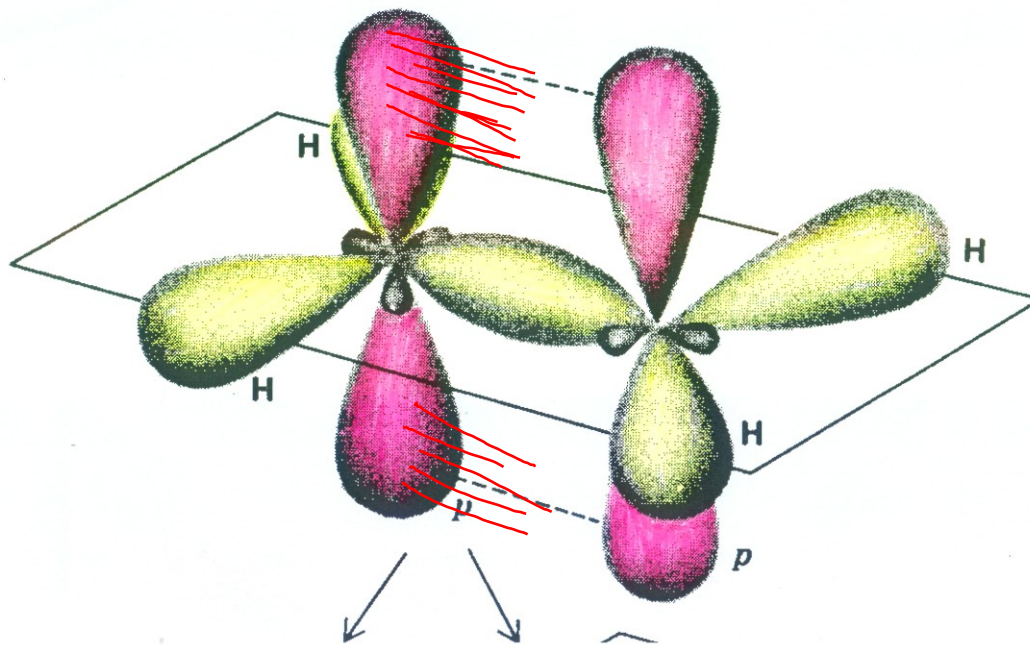
+ I effect



Bonding in organic molecules



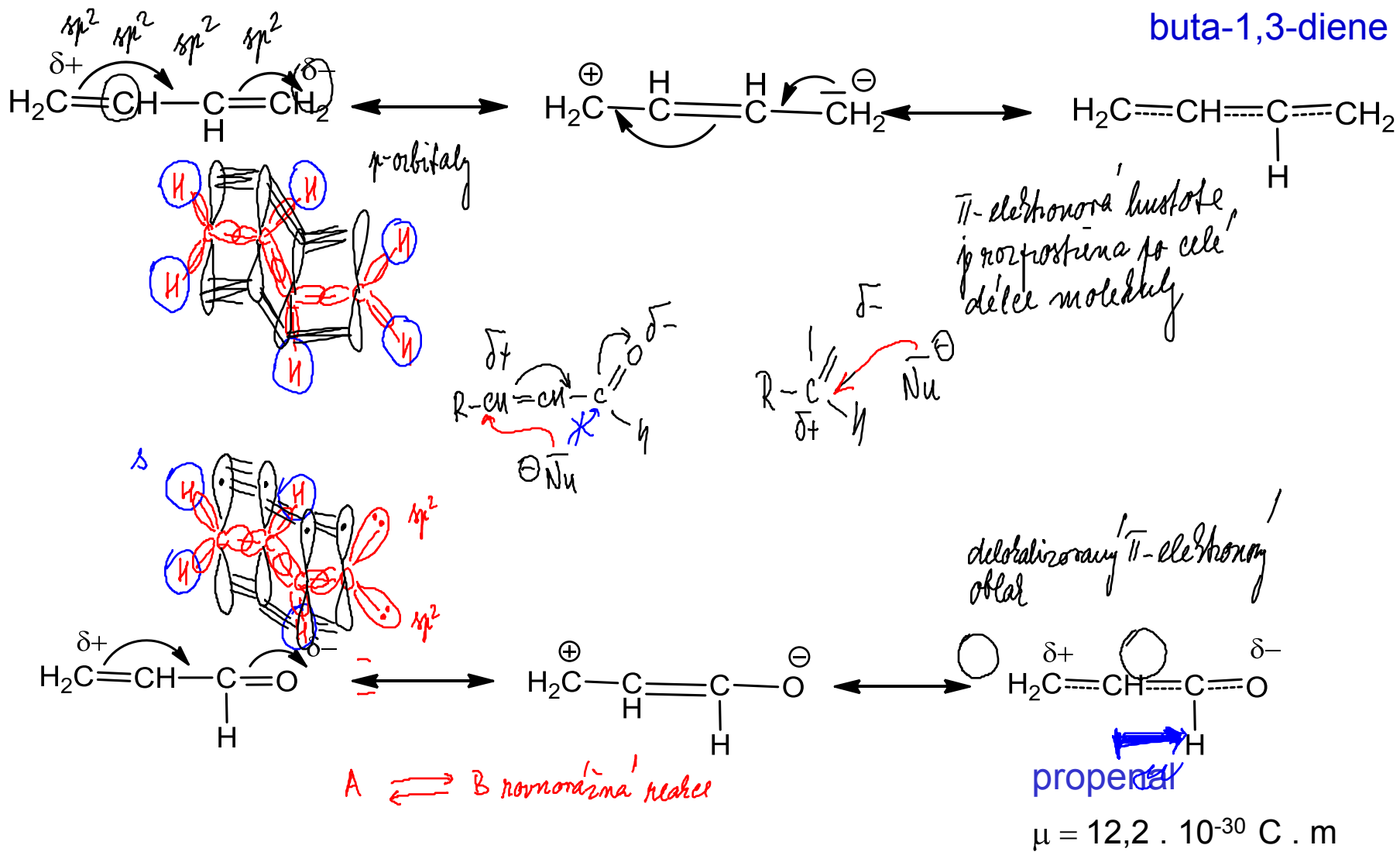
C atom in sp² hybrid state



Formation of π bond between carbon atoms in sp² hybrid state

Bonding in organic molecules

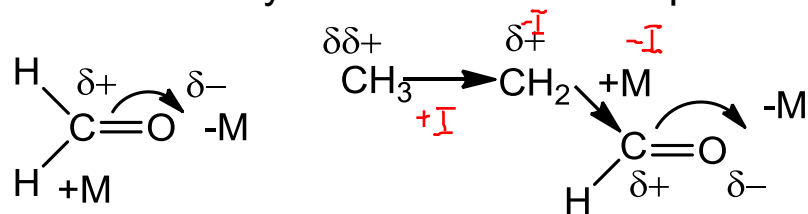
Molecules with conjugation – mesomeric (conjugation effect) + M , - M



Bonding in organic molecules

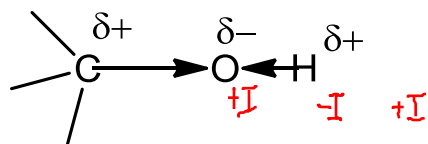
MESOMERIC (CONJUGATION) EFFECT

Mesomeric effect you can meet at multiple bonds (π – bonds)

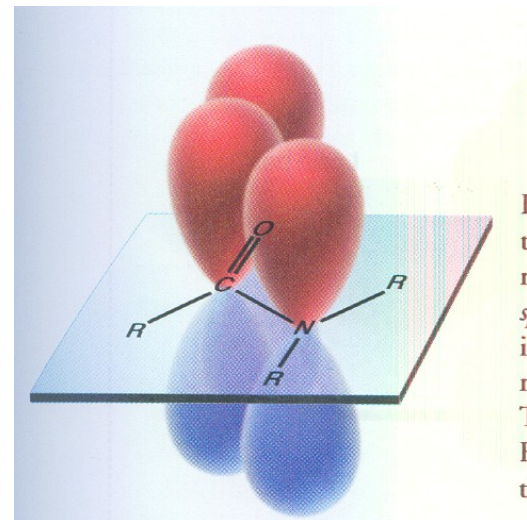


$$\mu = 7,6 \cdot 10^{-30} \text{ C} \cdot \text{m}$$

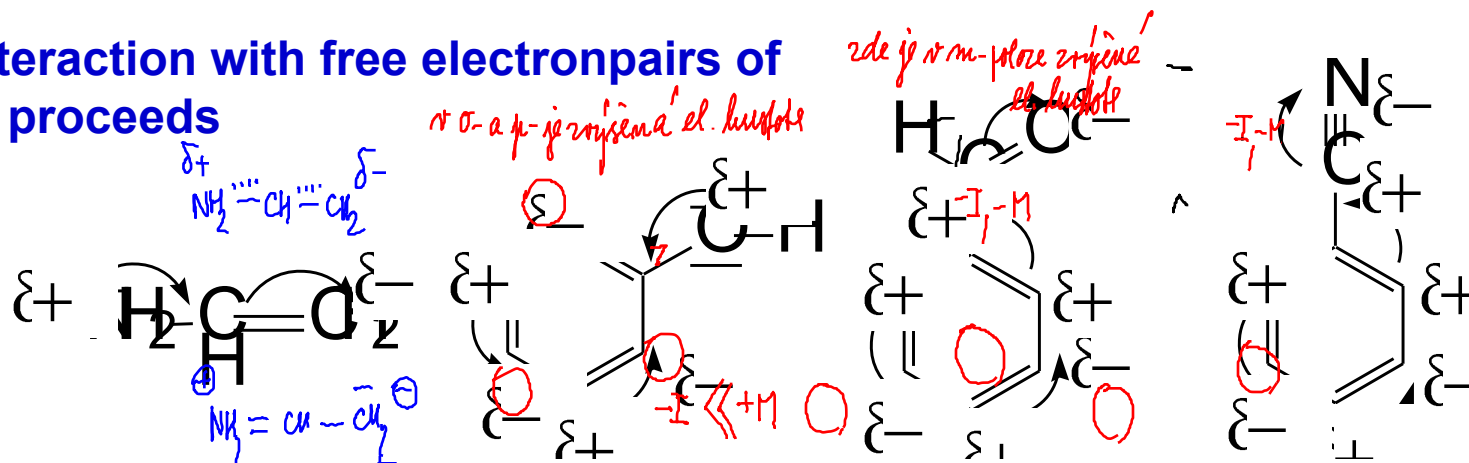
$$\mu = 9,0 \cdot 10^{-30} \text{ C} \cdot \text{m}$$



$$\mu = 2,46 \cdot 10^{-30}$$



Very often interaction with free electronpairs of heteroatoms proceeds



Bonding in organic molecules

Rules for working with resonance structures

Particular resonance structures are not real structures, they are imaginary only. The real structure consists from different structures they are trying to depict the real structure ; real structure is an resonance hybrid. Compounds like nitromethane, benzene or acetate anion have only one structure, which is not oscilating among the resonace structures. But way of their presentation at a paper may differ.

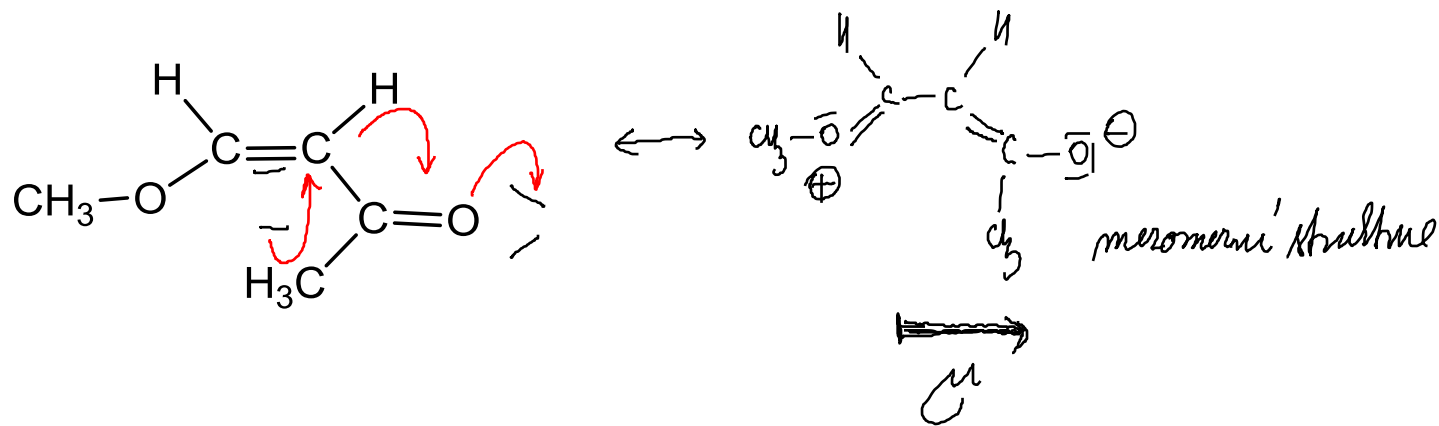
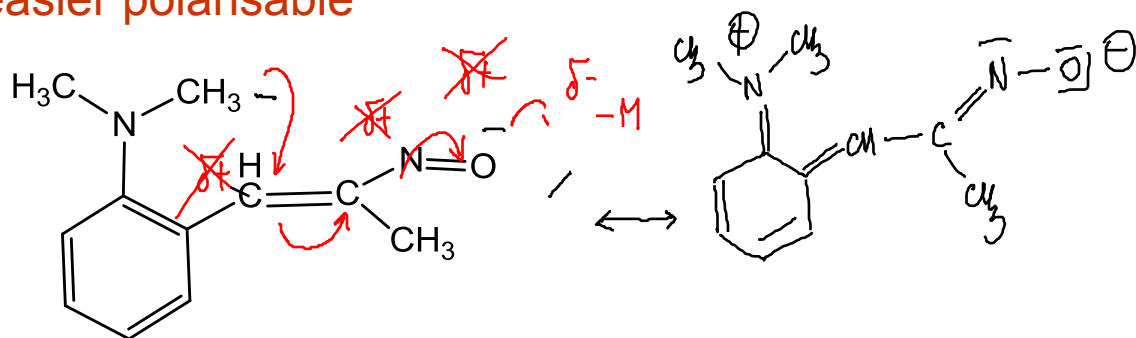
Resonance structures are differing by position of π - and non-bonding electrons only. When going from one resonance structure to another neither position nor hybridization of any of the atoms is changed. Thus, nitromethane has nitrogen atom in sp^2 hybridization and oxygen atoms keep in both resonance structures their position. They differ by position of π -electrons in N=O bond and by position of free electron pairs at oxygen atom. The electrons transfer when coming from one resonance structure to another is depicted by arrows. An arrow is always only showing transfer of electrons; no transfer of atoms. The point of arrow remembers that electron pairs are only formaly transfered from an atom or a bond towards to an atom or a bond in the point of arrow.

Bonding in organic molecules

When evaluate electron distribution in molecule, we are faced often to **simultaneous inductive and mesomeric effect**.

When the action is directed in the same direction, there is no problem.

In the case the effects have different direction, **mesomeric effect is the prevailing** - (effect at multiple bonds), because π electrons are more mobile - easier polarisable

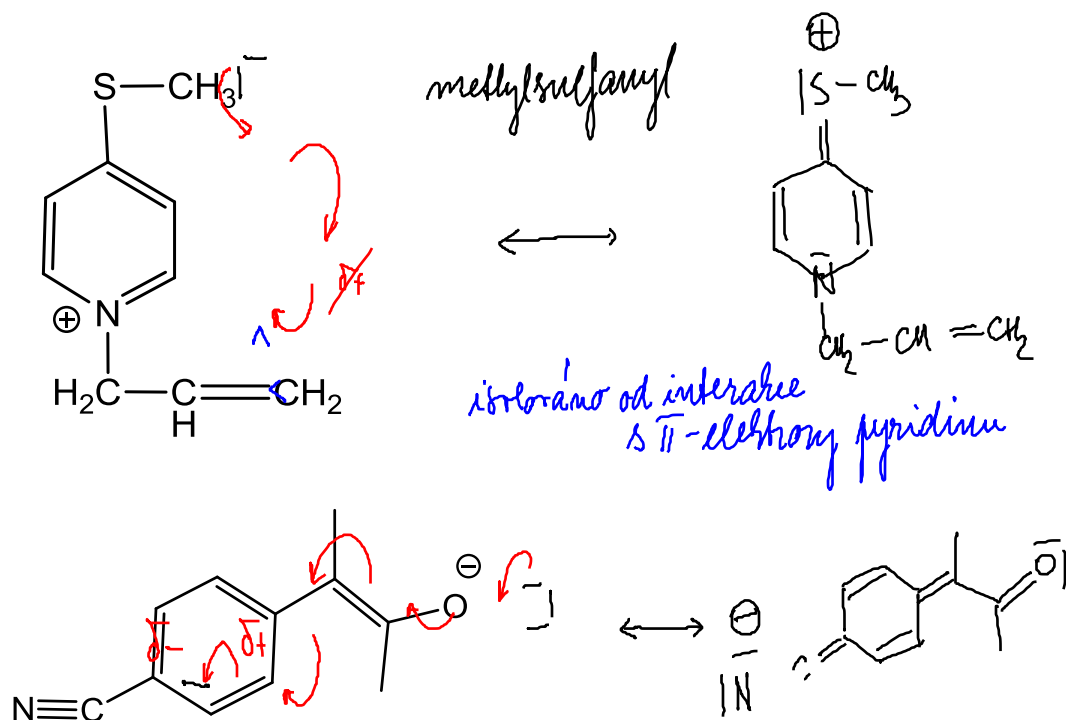


Bonding in organic molecules

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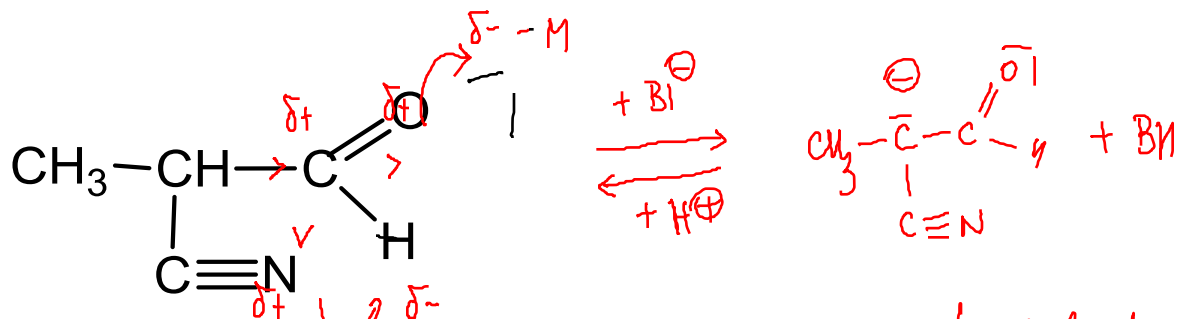
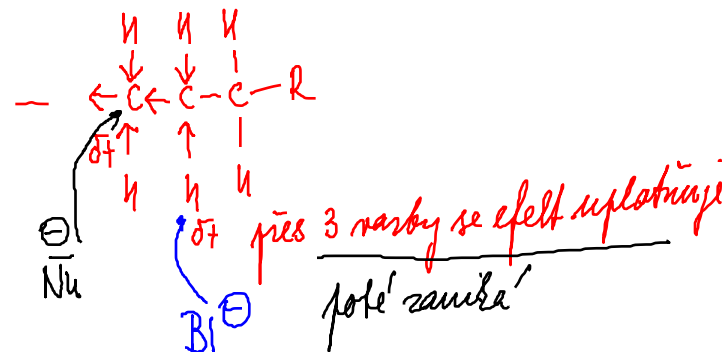
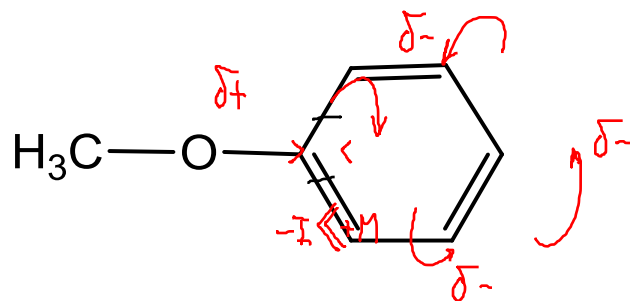
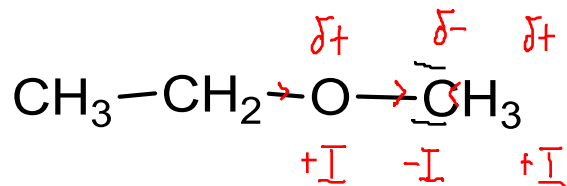
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Bonding in organic molecules

!!Attention!!

The same group can behave different way at aliphatic and aromatic ring!!

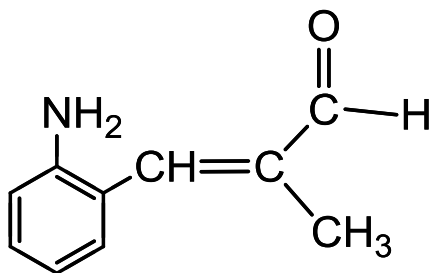
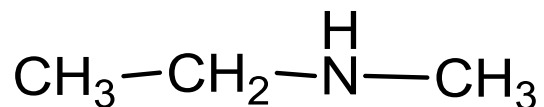
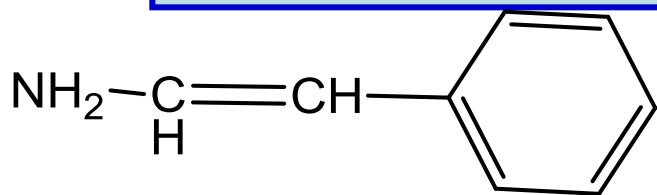


-M C-kyselina - kyselost je aktivována 2 akceptorými skupinami

Bonding in organic molecules

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Bonding in organic molecules

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