ORGANIC CHEMISTRY II

- Organic chemistry of hydrocarbon derivatives. Analysis of functional groups structure and their reactivity, influence of the neighbouring skeleton upon their reactivity and opposite influence of the certain functional group upon the hydrocarbon skeleton. Steroides and heterocyclic compounds in an overview.

  At the end of the course the student should understand reactivity of various functional groups and their influence upon the hydrocarbon skeleton with the final aim to deduce chemical behaviour of a complex molecule, which might be a centre of the interest.

References:

McMurry, John. *Organic chemistry*. 4th ed. Pacific Grove : Brooks/Cole publishing company, 1995. 1243 s. ISBN 0-534-23832-7.

Solomons, Graham T. W. *Organic chemistry*. 6th ed. New York : John Wiley & Sons, 1996. xxvii, 121. ISBN 0-471-01342-0.

J. Clayden, N. Greeves, S. Warren, P. Wothers. Organic Chemistry. Oxford University Press 2001

John McMurry. Organická chemie, český překlad. Vyd. 1. Praha : Vysoká škola chemicko-technologická v Praze *Organická chemie*., 2007. 1 sv. (ISBN 978-80-7080-637).

Červinka, Otakar. *Chemie organických sloučenin. Díl 1*. 1. vyd. Praha : Státní nakladatelství technické literatury, 1985. 1131 s.

Otakar Červinka, *Chemie organických sloučenin. Díl 2*.. 1. vyd. Praha : Státní nakladatelství technické literatury, 1987. 1052 s.

Potáček, Milan - Mazal, Ctibor - Janků, Slávka. Řešené příklady z organické chemie. Masarykova univerzita v Brně, 2008. 243 s. ISBN 80-210-2274-4.


LA CHE MA
pharmaceutica
diagnostica
chimica
PERIODICKÁ SOUSTAVA PRVKŮ
s
d
p
f
I.A
II.A
III.B
IV.B
V.B
VI.B
VII.B
VIII.B
VIII.B
VII.B
I.B
II.B
III.A
IV.A
V.A
VI.A
VII.A
VIII.A
hmotnostní číslo
značka (symbol)
protonové číslo
elektronová konfigurace
elektronegativita
český název
latinský název
Prvky
zásadotvorné silné
zásadotvorné slabé
amfoterní
kyselinotvorné slabé
kyselinotvorné silné
inertní
umělé
Skupenství prvků (při 30 °C):
He – plynné
Hg – kapalné
Fe – pevné
* LANTHANOIDY
** AKTINOIDY

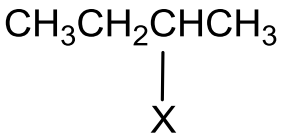
Electronegativity of various atoms by Pauling

H 2,20						
Li 0,98	Be 1,57	B 2,04	C 2,55	N 3,04	O 3,44	F 4,00
Na 0,93	Mg 1,31	Al 1,51	Si 1,90	P 2,19	S 2,58	Cl 3,16
				As 2,18	Se 2,55	Br 2,96
						I 2,66

Halogen derivatives

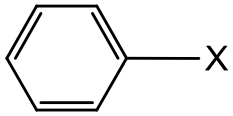
according their reactivity we can summarize the types of halogen derivatives by the way the halogen at the molecule is bound to the hydrocarbon skeleton

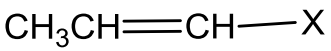
Halogenides with halogen at carbon **sp^3**



„normal“ reactive

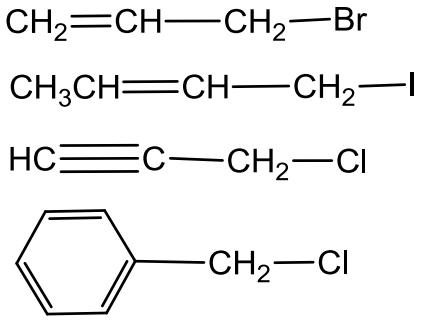
Halogenides with halogen at carbon **sp^2**





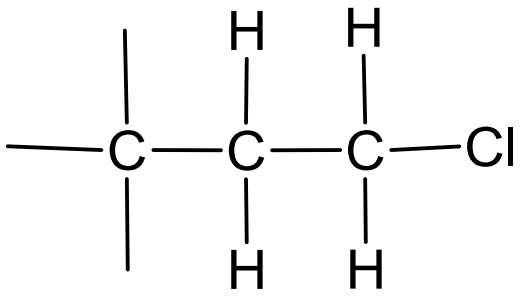
nonreactive

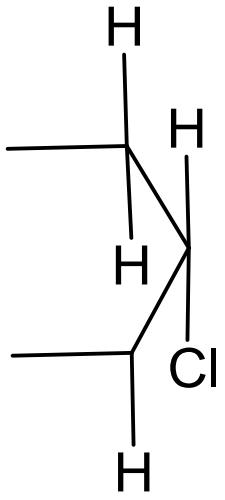
Halogenides with halogen at carbon **sp^3** in neigbourhood of carbon **sp^2** or **sp**



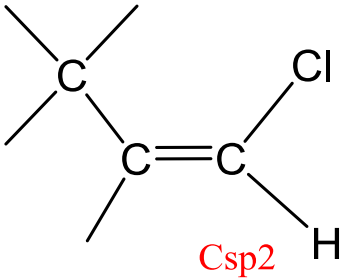
very reactive

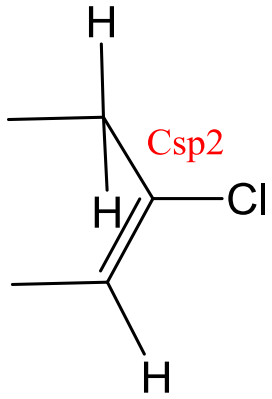
HALOGEN DERIVATIVES

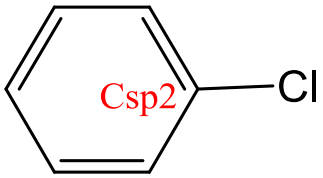




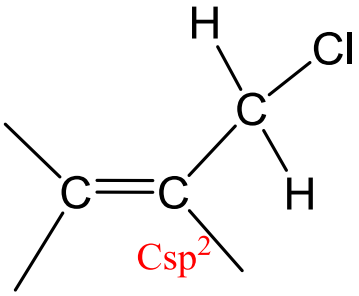
HALOGEN DERIVATIVES

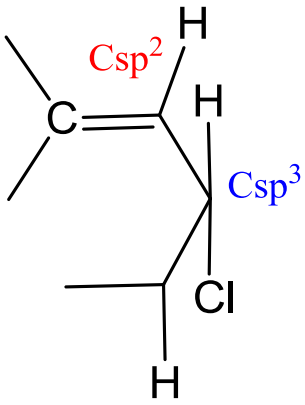


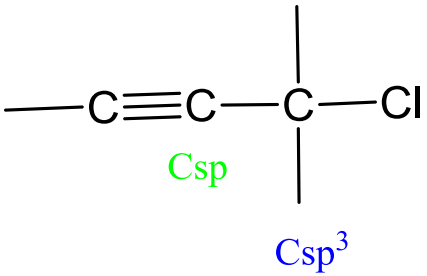




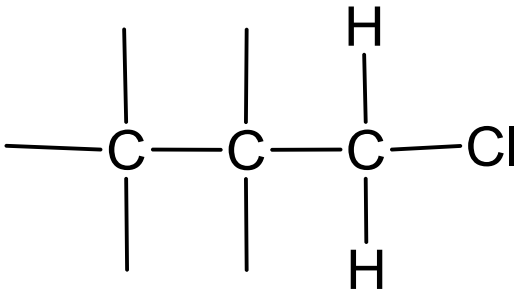
Csp^3 HALOGEN DERIVATIVES

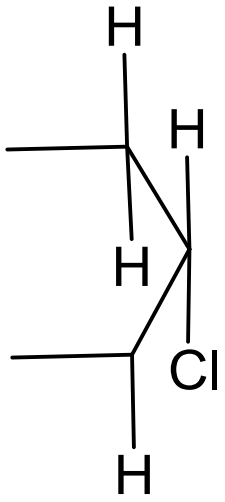






HALOGEN DERIVATIVES





HALOGEN DERIVATIVES

	C - F	C - Cl	C - Br	C - I
Dipole moment [C. m.10^{-30}]	4,69	4,86	4,56	3,96
Bond energy [kJ/mol]	447	339	280	221
Polarisability [10^{24}.cm^{-3}.mol^{-1}]	0,81	5,84	8,74	13,95

Overview of some hard and soft acids and bases

	Bases	Acids
HARD	H_2O, HO^-, F^-, Cl^- CH_3COO^-, SO_4^{2-}, NO_3^- ClO_4^-, CO_3^{2-}, ROH, R_2O, NH_3, RNH_2	H^+, Li^+, Na^+, K^+, Al^{3+}, Fe^{3+} $AlCl_3$, BF_3, $(RO)_3B$ R_3C^+, RCO^+, NC^+
SOFT	RSH, RS^-, R_2S I^-, SCN^-, $S_2O_3^{2-}$ R_3P, $(RO)_3P$, CN^-, RNC, alkeny benzen, H^-, R^-	Cu^+, Ag^+, Hg^+ CH_3Hg^+, BH_3 RS^+, I^+, Br^+ I_2, Br_2 chinony, karbeny, kovy

Basicity and nucleophility comparison

Swain – Scott equation

$$\log \frac{k}{k_o} = s \bullet n$$

$$CH_3Br + H_2O \xrightarrow{k_o} CH_3OH + HBr$$

$$CH_3Br + NuH \xrightarrow{k} CH_3OH + HBr$$

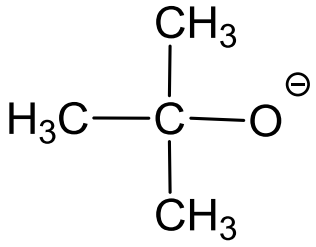
k = rate constanta for reaction of brommethane with a nucleophile with nucleophility n

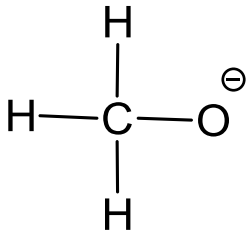
k_o = rate constant for reaction of brommethane with water [$n_{(H2O)} = 0$]

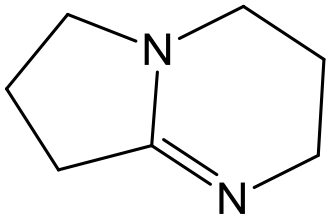
s = sensitivity of substrate to nucleophilic attack (dependent upon the structure, pro brommethane s=1)

Reagent	Nucleophility	Basicity
H_2O	**0,0**	**0,0**
F^-	**2,0**	**4,9**
Cl^-	**3,0**	**- 3,0**
Br^-	**3,8**	**-6,0**
I^-	**5,0**	**-9,0**
HO^-	**4,2**	**17,5**
CH_3COO^-	**2,7**	**6,5**
CN^-	**5,1**	**-9,0**
HS^-	**5,1**	**14,7**

Basicity

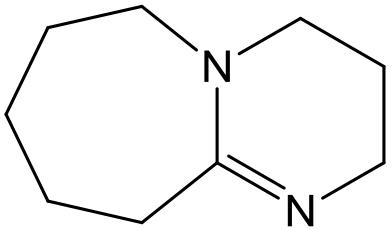






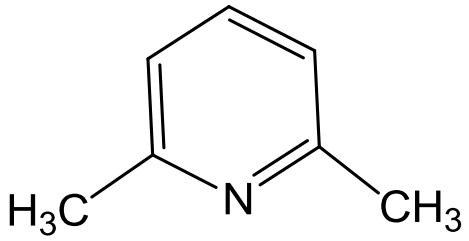
DBN

1,5-diazabicyclo[4.3.0]non-5-ene

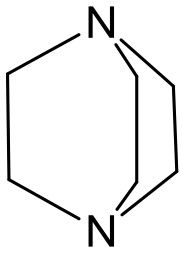


DBU

1,5-diazabicyclo[5.4.0]undecene



2,6-dimethylpyridin



DABCO

1,4-diazabicyclo[2.2.2]octane