esf european social fund in the czech republic
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OP Education for Competitiveness
INVESTMENTS IN EDUCATION DEVELOPMENT

Innovation and Development of Study Field Nanomaterials at the Technical University of Liberec

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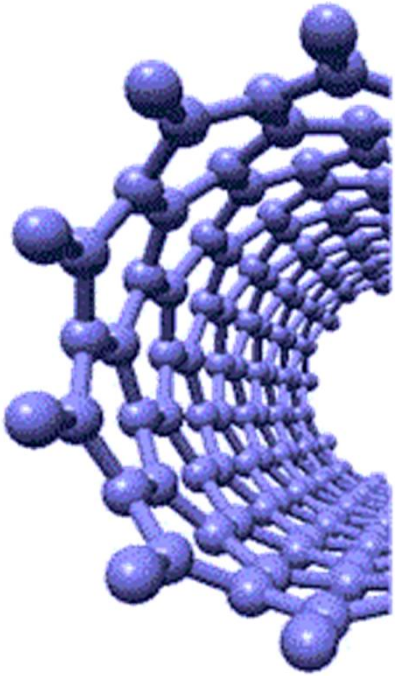

These materials have been developed within the ESF project: Innovation and development of study field Nanomaterials at the Technical University of Liberec

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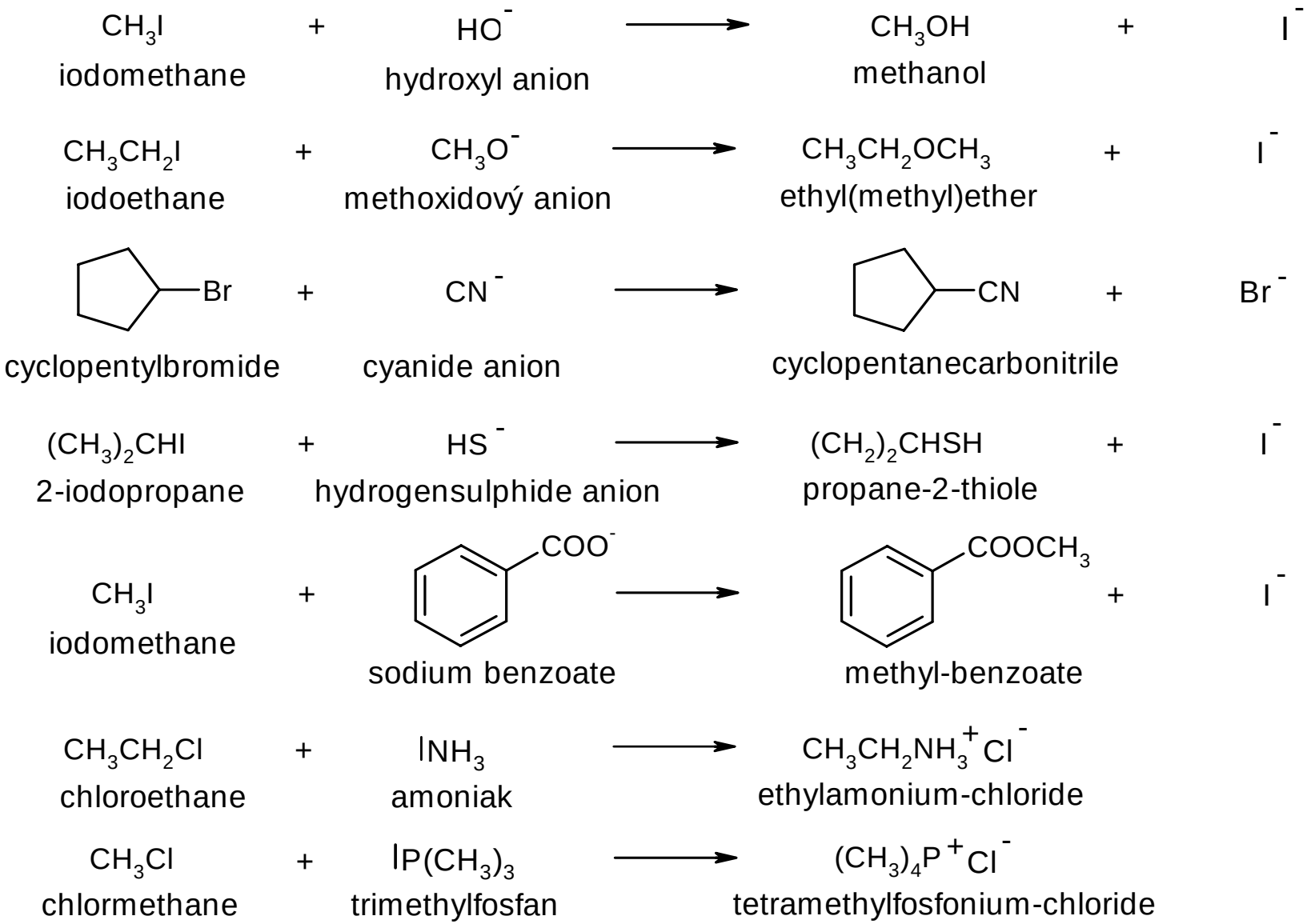
Halogenderivatives- Bond lenghts and strenghts of C-X bond

Halogenmethane	Bond lenght (pm)	Disociation energy ($kJ.mol^{-1}$)
CH_3F	138,5	460
CH_3Cl	178,4	356
CH_3Br	192,9	297
CH_3I	213,9	238

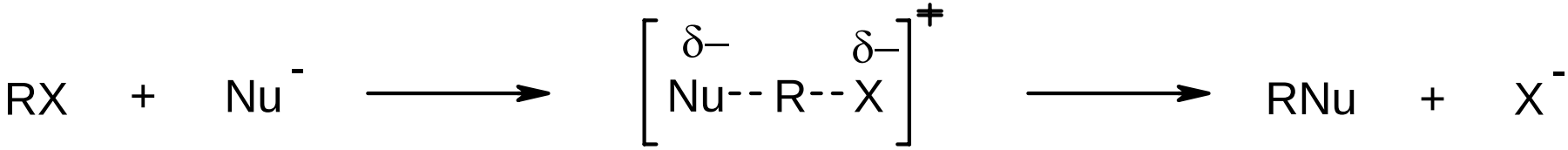
Organic Chemistry – functional groups



Halogenderivatives- Nucleophillic substitution – mechanism

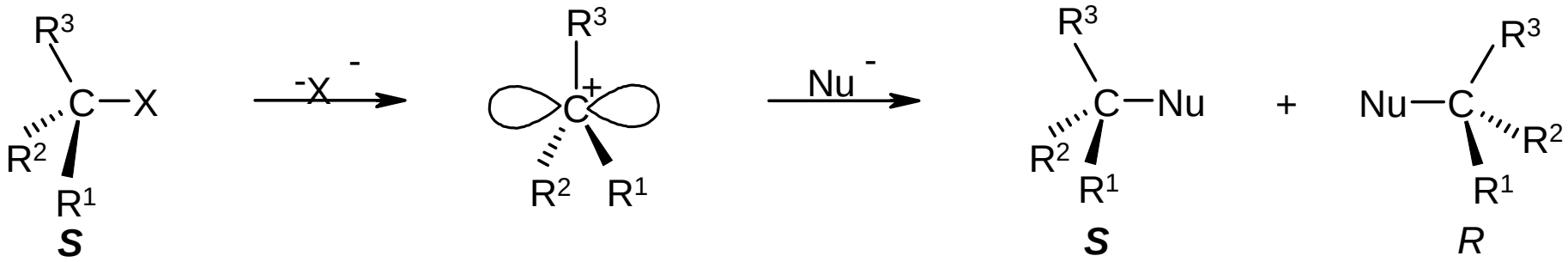
S_N1

S_N2



Halogenderivatives- Nucleophillic substitution – stereochemistry

S_N1



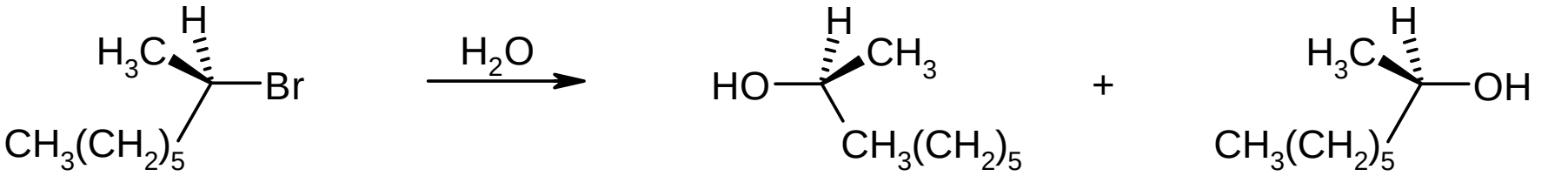
chiral,
optically active

planar, achiral
optically inactice

racemate
mixture 1:1 of both isomers

Halogenderivatives- Nucleophillic substitution – stereochemistry

S_N1



(*R*)-2-bromooctane

(*S*)-octane-2-ol (83%)

(*R*)-octane-2-ol (17%)

Halogenderivatives - Nucleophillic substitution – S_N1 solvolysis

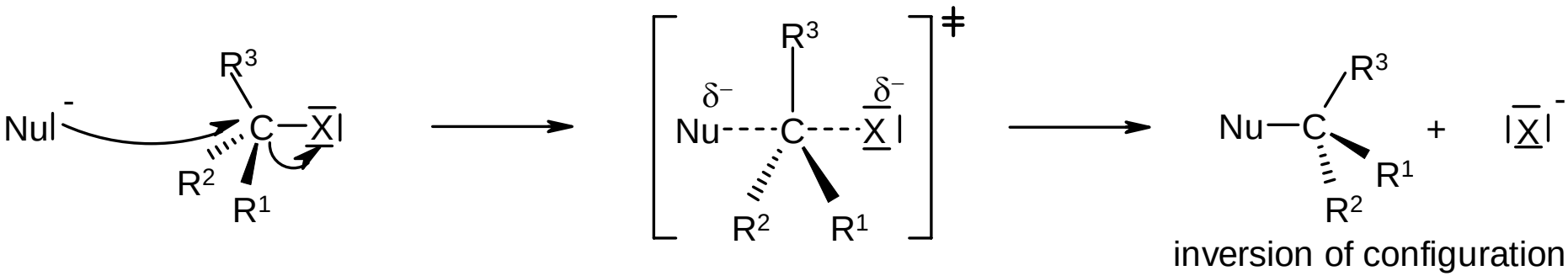
Alkylbromide	**Structure**	**Type**	**Relative velocity**
Bromomethane	CH_3Br	methyl	1
Bromoethan	CH_3CH_2Br	Primary	2
Isopropylbromide	$(CH_3)_2CHBr$	Secondary	43
Tert-butylbromide	$(CH_3)_3CBr$	Tertiary	100 000 000

Halogenderivatives - S_N1 the role of solvent

solvent	**dielectric constant ε**	**relative velocity**
acetic acid	6	1
methanol	33	4
formic acid	58	5000
water	78	150000

Halogenderivatives- Nucleophillic substitution – stereochemistry

S_N2

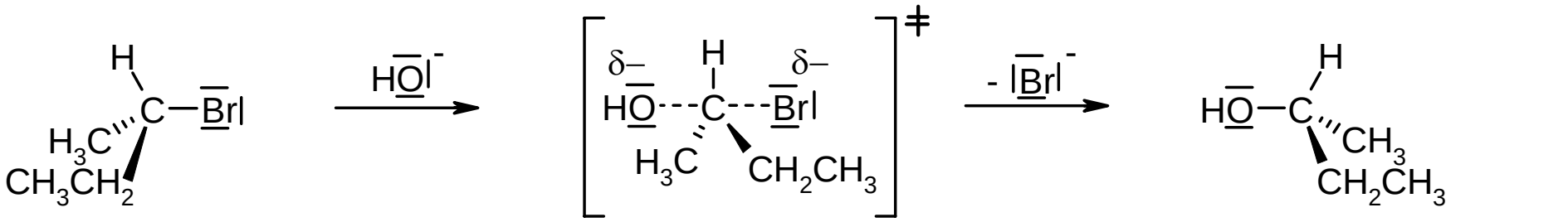


inversion of configuration

Transition state

Halogenderivatives- Nucleophillic substitution – stereochemistry

S_N2



(S)-2-bromobutane

transition state

(R)-butane-2-ol

inversion of configuration

Halogenderivatives- S_N2: Structure of halogenderivative

. S_N2

R-Br	Structure	Type	Rel. velocity
Methylbromide	CH_3Br	methyl	221000
Ethylbromide	CH_3CH_2Br	primary	1350
Isopropylbromide	$(CH_3)_2CHBr$	secondary	1
Tert-butylbromide	$(CH_3)_3CBr$	tertiary	non-measureable

Halogenderivatives- S_N2: Nucleophilicity of reagent

	Nucleophile	**Rel. velocity**
Very strong	I^-, HS^-, RS^-	$> 10^5$
Strong	Br^-, HO^-, RO^-, CN^-, N_3^-	10^4
Average	NH_3, Cl^-, F^-, RCO_2^-	10^3
Weak	H_2O, ROH	1
Very weak	RCO_2H	10^{-2}

Halogenderivatives- S_N2: leaving group

Conjugated acid		pK_a
Hydrogen iodide	HI	-5,2
Hydrogen bromide	HBr	-4,7
Hydrogen chloride	HCl	-2,2
Sulfuric aciíd	H_2SO_4	-5
Methanesulphonic acid	CH_3SO_3H	-1,2
Hydroxonium ion	H_3O^+	-1,7
Hydrogen fluoride	HF	3,2
Acetic acid	CH_3CO_2H	4,7
Methanol	CH_3OH	15,5
Water	H_2O	15,7
Amoniak	NH_3	35

Halogenderivatives- S_N2: solvent

solvent		**Dielectric constant ε**	**Relativní rychlost**
Methanol	CH_3OH	32,6	1
Water	H_2O	78,5	7
DMSO	$(CH_3)_2S{=}O$	48,9	1300
DMF	$HCON(CH_3)_2$	36,7	2800
Acetonitrile	CH_3CN	37,5	5000