the software I

ually shows an alternative view.

propane-1,2-diol

ethanal

pot works like a 'play' or 'reveal' button.

help - how to use the software II

Reset:

To 'run' a slide again press reset. You use 'reset' often - certainly more than you would repeat showing a PowerPoint slide. When you click reset, the slide looks as if you had just arrived.

Slider:

Look for a slider if there are no hotspots. It advances a sequence and also allows you to repeat something - drag this slider. Often a red hotspot nearby does exactly the same job as a slider. Alternatively to rewind the action, press 'reset'.

help - using 3D-models - Jmol

3D models help to remind us that chemistry is anything but flat - though there are other reasons. We need to compare isomers or show charge distribution and show you which molecules really are flat!

When you spot an "Jmol" model (a black background) you can interact with it in useful ways. The models are 'industry standard' so the skills below are really useful in the world of chemistry. The instructions show how to find information locked in the model.

To rotate the model, press the mouse button and drag across the screen.

To zoom in or out - hold down SHIFT key, press the left button and move the mouse down / up to zoom.

help - safe thinking and save thinking

- Thinking about what happens in a chemical reaction, how to make it happen safely and why it happened are big ideas in chemistry. To help the thinking, this compendium provides pictures of 'structures', 'electrons', 'orbitals' and 'reactions'. In a healthy diet of classroom studies and hands-on laboratory work, this software is a thinking supplement.
- Although we show bonds, electrons and reagents, everything here is a picture! Real bonds are not dashes, electrons are not dots and you cannot isomerise butane by plucking its CH_3 group.
- Equally, C_6H_6 is not 'benzene'. We show models, bottles, formulae and lab glassware to raise questions about doing chemistry on a computer. Study the screen and discuss what is not real, what is not safe and also why they are without hazard signs.
- Do not think to do this chemistry without having an expert assess the risks or adjust reagents and apparatus to minimise them.

Back | Next

help - to the student

- Welcome to this compendium of models, mechanisms and organic chemistry. It's meant to be used for talking about ch Practising how to do that is going to help you lots.

Top tips:

- Work through a slide, list its points and then check the text
- Imagine you're a teacher explaining a screen. Go through e the words that go with the pictures.
- Work through a topic and stop. Write down the headings an made.
- If you're stuck, see what your chemistry book says about th If you are using this to catch up on missed work, again have
- Maximum use is 15 minutes. If you're just whizzing through, instead.
- There is a help page on **Using the 3D-Models.**

e - homologous series

CH_3-CH_3 C_2H_6

hydrocarbons - introduction

ethane saturated aliphatic hydrocarbon

alkanes - cycloalkanes - structure

cyclopentane C_5H_{10}

alkanes - IUPAC nomenclature

citrus fruit

2-hydroxy-1,2,3-propanetricarboxylic acid *'citric acid'*

'aspirin'

2-ethanoyloxy benzenecarboxylic acid *'aspirin'*

alkanes - IUPAC nomenclature - parent name

number of C atoms	structural formula	name	alkyl group
1	CH_4	methane	[-H] methyl
2	CH_3CH_3	ethane	[-H] ethyl
3	$CH_3CH_2CH_3$	propane	[-H]
4	$+CH_2$		
5			
6			

omenclature - longest chain

3-methylpentane

alkanes - IUPAC nomenclature - numbering chains

4-methylhexane

alkanes - IUPAC nomenclature - substituents

2-methylpentane

alkanes - IUPAC nomenclature - exercise

2-methylpentane

?

?

alkanes - reactions - combustion

methane

normal air

$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$

methane carbon dioxide

- chlorination of methane

UV lamp

ethane gas

alkanes - free radical substitution - chlorination

CH_3Cl

Cl_2

alkanes - free radical substitution - chlorination - summary

$CH_4 + Cl_2 \xrightarrow{\text{ultra-violet}} CH_3Cl + HCl$ (chloromethane)

$CH_3Cl + Cl_2 \xrightarrow{\text{ultra-violet}}$

$CH_2Cl_2 + Cl_2 \xrightarrow{\text{ultra-violet}}$

$CHCl_3 + Cl_2 \xrightarrow{\text{ultra-violet}}$

alkanes - free radical substitution - chain reaction

$CH_4 + Cl_2 \longrightarrow CH_3Cl + HCl$

initiation

propagation

termination

alkanes - free radical substitution - exercise

$CH_4 + Cl_2 \longrightarrow CH_3Cl$

$Cl\bullet$ $\bullet CH_3$ CH_3Cl

initiation $Cl-Cl \xrightarrow{\text{ultra-violet}} Cl\bullet$

propagation $CH_4 + Cl\bullet \longrightarrow$; $+ Cl_2 \longrightarrow$

termination $+ \longrightarrow Cl_2$; $+ \longrightarrow$; $+ \longrightarrow C_2H$

lical substitution - bromination - exercise

UV lamp

hexane

isomerism - structural isomerism - introduction I

$CH_3-CH_2-CH_2-CH_3$ butane C_4H_{10}

$CH_3-CH_2-CH_2-CH_3$ butane C_4H_{10}

isomerism - structural isomerism - introduction II

C_6H_{12} C_3H_8 C_3H_7OH

$CH_3-CH_2-CH_3$ propane C_3H_8

$CH_3-CH_2-CH_3$ propane C_3H_8

isomerism - structural isomerism - exercise - pentane

$CH_3-CH_2-CH_2-CH_2-CH_3$ pentane C_5H_{12}

$CH_3-CH_2-CH_2-CH_2-CH_3$ pentane C_5H_{12}

$CH_3-CH_2-CH_2-CH_2-CH_3$ pentane C_5H_{12}

isomerism - structural isomerism - chain isomerism

$CH_3-CH_2-CH_2-CH_3$ butane C_4H_{10}

CH_3-CH butane

tural isomerism - position isomerism

CH_2-O-H C_3H_7OH

propan-1-ol C_3H_7OH

isomerism - structural isomerism - exercise

$C_6H_4Cl_2$ 1,4-dichlorobenzene

$C_6H_4Cl_2$ 1,4-dichlorobenzene

$C_6H_4Cl_2$ 1,4-dichlorobenzene

isomerism - structural isomerism - functional group isomerism

CH_3-CH_2-O-H C_2H_6O ethanol

CH_3-CH_2-O-H C_2H_6O ethanol

isomerism - stereoisomerism - geometric isomerism - bond rotation

$CH_3-CH_2-CH_2-CH_3$ C_4H_{10} butane

$CH_3-CH_2-CH_2-CH_3$ C_4H_{10} butane

isomerism - stereoisomerism - geometric isomerism - restri

$CH_3-CH=CH-CH_3$ C_4H_8 but-2-ene

CH_3-CH C_4H_8

eoisomerism - geometric isomerism

CH—CH₃
cis-but-2-ene
t: 134 K

CH₃—CH=CH—CH₃
(E)-2-butene
trans-but-2-ene
melting point: 168 K

isomerism- stereoisomerism - geometric isomerism - exercise

(Z)
(E)

isomerism - stereoisomerism - geometric isomerism - retinal

C₂₀H₂₈O
C₂₀H₂₈O

isomerism - stereoisomerism - geometric isomerism - fluoroethene

H₂C=CHF
C₂H₃F
fluoroethene

FHC=CHF
C₂H₂F₂
1,2-difluoroethene

isomerism - stereoisomerism - optical isomerism - chi

chiral carbon
CH₃
CH₃CH₂NH₂
ethylamine
CH₃CHNH
2-aminopropan

oisomerism - optical isomerism - non-superimposable

NH₂
c acid (alanine)

COOH
NH₂
H
CH₃
2-aminopropanoic acid (alanine)

isomerism - stereoisomerism - optical isomerism - enantiomers

mirror image
bromochloroiodomethane
bromochloroiodomethane

isomerism - stereoisomerism - optical isomerism - optical activity

lactic acid
lactic acid mirror image
'equimolar racemic' mixture

isomerism - stereoisomerism - optical isomerism - limonene

limonene

alkanes - fuels - formation of oil

Sandstone
plankton / clay

ractional distillation

gas C₁₋₄ (<5 °C)
lubricating oil
C₂₀₋₅₀
acuum
illation

alkanes - fuels - fractional distillation - exercise

carbon count	name	boiling point °C	viscosity	ignition	use
C_1-C_4	diesel oil	↑↑			domestic heating
C_5-C_{10}	paraffin	↑↑↑↑	less viscous	less flammable	car fuel/ plastics
C_{10}-C_{16}	bitumen	↑↑↑			jet engine fuel
C_{14}-C_{20}	lubricating oil	↓↓	more viscous	more flammable	diesel engine fuel
C_{20}-C_{50}	petrol/ naphtha	↑			engine lubrication
>C_{70}	gas	↓			roof and road covering

alkanes - fuels - octane rating

high 'octane' number = 100
?
low 'octane' number = 0
?

alkanes - fuels - catalytic converter

spark plug
O_2 N_2 fuel
NO_x H_2O

alkanes - fuels - supply and demand

percentage of total
demand
supply
gas
petrol & naphtha
paraffin
diesel o

omerisation of alkanes for fuel

zeolite catalyst
temperature 500 °C pressure <1 atmospheres
furnace

alkanes - fuels - cracking alkanes for fuel

zeolite catalyst (aluminosilicate) 500 °C
naphtha

Carbon compounds - thermal cracking of alkanes

ethane
70 atmospheres at 1000 °C

Carbon compounds - reforming alkanes for fuel

octane
straight chain alkane 'low octane rating'
platinum on aluminium oxide 500 °C at 20 atmospheres

alkanes - fuels - air pollution

cid rain

alkenes - structure - homologous series

H H H
H—C=C—C—H
H

propene $CH_2=CH-CH_3$ C_3H_6

alkenes - IUPAC nomenclature

number of C atoms	structural formula	name
2	$CH_2=CH_2$	ethene
3		
4		
5		
6		

alkenes - IUPAC nomenclature

number of C atoms	structural formula	name
2	$CH_2=CH_2$	ethene
3	$CH_2=CHCH_3$	propene
4	$CH_2=CHCH_2CH_3$	but-1-ene
5	$CH_2=CHCH_2CH_2CH_3$	pent-1-ene
6	$CH_2=CHCH_2CH_2CH_2CH_3$	hex-1-ene

alkenes - IUPAC nomenclature - exercise - cis and trans

cis-but-2-ene
cis-hex-3-ene

oints

molecular size
alkene boiling points

alkenes - addition of bromine

ethene gas
bromine in tetrachloromethane

alkenes - addition of bromine - mechanism

ethene gas

alkenes - addition of hydrogen

nickel catalyst
silver catalyst
tungsten catalyst

alkenes - addition of hydrogen - fats

H_2
Ni, Pt or Pd
an unsaturated fatty acid (melting point +10° C)

of hydrogen halide

alkenes - addition of hydrogen halide - mechanism

bromoethane

alkenes - addition of hydrogen halide - Markovnikov's rule

carbocation intermediates

alkenes - addition of water

phosphoric acid catalyst

high pressure

ethene

alkenes - addition with concentrated H_2SO_4 - mechanism

n polymerisation

alkenes - oxidation

propene gas

acidified potassium manganate(VII) solution

propene

ethene

bonding in methane - hybridisation - bond angle

bonding in methane - hybridisation - carbon electron configuration

carbon : ground state electron configuration

bonding in methane - hybridisation - exercise

Orbitals

ane - hybridisation - exercise

carbon: ground state electron configuration

bonding in ethene - hybridisation - bond angle

ethene

bonding in ethene - hybridisation - carbon electron configuration

carbon : ground state electron configuration

bonding in benzene - hybridisation

bonding in ethyne - hybridisation - bond angle

- hybridisation - carbon electron configuration

polymers - addition polymers II - examples

monomer

polymer

ethene

'ethylene'

polymers - addition and condensation

addition polymerisation

condensation polymerisation

polymers - addition polymers I - free radical

conditions

temperature in °C

pressure in atmospheres

polymers - natural polymers - rubber

es - stereoisomers

isotactic

syndiotactic

atactic

polymers - condensation polymers - polyester

formation of a polyester

polymers - condensation polymers - polyamide

formation of a polyamide

polymers - making nylon - phenol

reduction

phenol

cyclohexanol

polymers - bakelite - phenol

ns - wool

polymers - elastomer

thermosetting

elastomer

analysis and detection - mass spectrometry - fragments

electron gun

relative abundance %

analysis and detection - mass spectrometer

electron gun

negative plates

electromagnet

Magnetic field strength

High

Medium

Low

vacuum pump

detector

amplifier

analysis and detection - mass spectrometry - exercise

relative abundance / %

Clues:

tection - infrared spectroscopy

analysis and detection - infrared spectroscopy - fingerprint region

transmittance %

wavenumber cm⁻¹

propan-1-ol

propan-2-ol

ethanol

analysis and detection - infrared spectroscopy - use of nujol

transmittance %

phenol + nujol

wavenumber cm⁻¹

phenol

chloroethane

N-phenylethanamide

analysis and detection - infrared spectroscopy - interpreting spectra

benzoic acid

paracetamol

transmittance %

wavenumber cm⁻¹

table

analysis and detection - infrared spectroscopy - exercise

transmittance / %

wavenumber / c

ection - low resolution NMR

signal height

butane

chemical shift δ / ppm

analysis and detection - high resolution NMR

radio frequency generator

signal height

ethyl ethanoate

ethanol

chemical shift δ / ppm

analysis and detection - NMR - exercise

chemical shift δ / ppm

Clues:

reactions - organic synthesis - exercise

two steps

three steps

starting compound

desired compound

KOH - ethanol - heat

KOH - water - heat

NH₃ - ethanol - heat

KCN - ethanol - heat

K₂Cr₂O₇ - acid - heat

K₂Cr₂O₇ - acid - heat

acid - heat

alkali - heat

CH₃CH₂Br

halogenoalkane

CH₃COOH

carboxylic acid

reactions - organic synthesis - pathways

alcohol

alkene

halogeno alkane

aldehyde

ketone

ester

alkane

amine

nitrile

ologous series - structure

—CH₂—OH

C₂H₅OH

alcohols - classification I

propan-1-ol

CH₃—CH₂—CH₂—O—H

alcohol

alcohols - classification II

propan-1-ol

—O—H

alcohols - classification - exercise

Examples

CH₃—CH(CH₃)—CH₂—OH

Name and classify the four examples

boiling points - intermolecular forces

pentane

heat

1-but

he

king the RO-H bond - reaction with sodium

sodium

ethanol

pH-meter

alcohols - breaking the RO-H bond - esterification

ethanol + ethanoic acid

alcohols - breaking the RO-H bond - with acyl chlorides

ethanol

ethanoyl chloride

ethyl ethanoate

ethyl ethanoate

alcohols - halogenation with hydrochloric acid & ZnCl₂ catalyst

characteristic test

ROH + HCl $\xrightarrow{\text{anhydrous } ZnCl_2}$ RCl + H₂O

alcohols - breaking the R-OH bond with PCl₅

characteristic test

CH₃CH₂OH + PCl₅ ⟶ CH₃CH₂Cl + PO

chloroethane

ing the R-OH bond - with phosphorus and iodine

2P + 3I₂ ⟶ 2PI₃

3CH₃CH₂OH + PI₃

3CH₃CH₂I + H₃PO₃

ethanol

iodine

alcohols - breaking the R-OH bond - with hydrogen halide

carrying out the reaction

sodium bromide

mix

reflux

distill

purify

dry

redistill

alcohols - breaking the R-OH bond - elimination of water using heat

mineral wool soaked in ethanol

Al₂O₃

heat

water

alcohols - elimination of water using concentrated acid

NaCl(aq)

cyclohexanol

concentrated H₃PO₄

cyclohexene

mix

distill

wash

dry

redistil

alcohols - elimination of water - mechanism

CH₃CH₂OH $\xrightarrow[180\,^{\circ}C]{\text{excess conc.}H_2SO_4}$ CH₂ = CH₂

ethene

ation - structure

2-methyl propan-2-ol

acidified $KMnO_4$

acidified $K_2Cr_2O_7$

alcohols - oxidation to aldehyde

propan-1-ol

excess oxidising agent

excess alcohol

alcohols - carboxylic acids from alcohols and aldehydes

$CH_3CH_2OH + 2[O] \xrightarrow{Cr_2O_7^{2-}/H^+} CH_3COOH + H_2O$

ethanol

primary alcohol

ethanoic acid

carboxylic acid

alcohols - triiodomethane reaction

characteristic test

triiodomethane

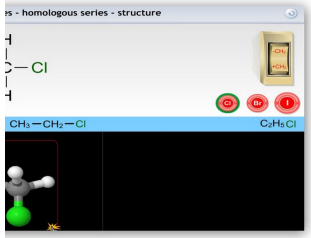
I₂ in NaOH

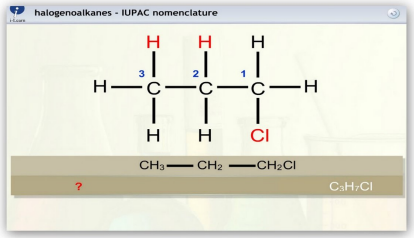
methanol

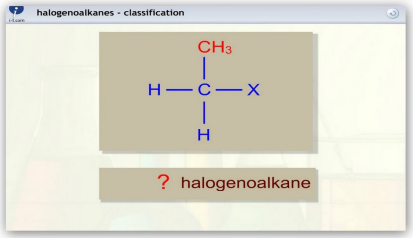
NaOI

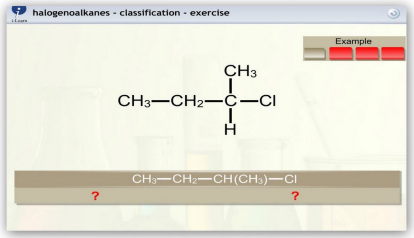
ethanol

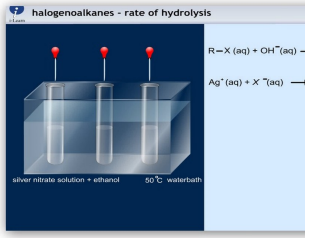
alcohols - triiodomethane reaction - exercise

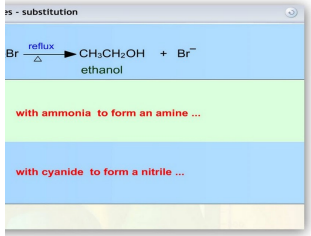


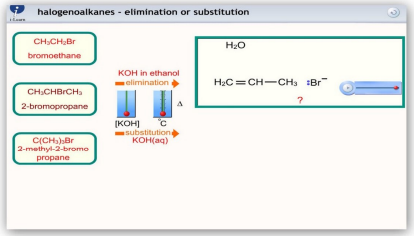


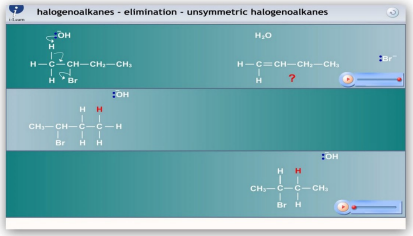


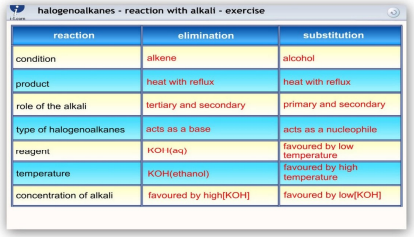




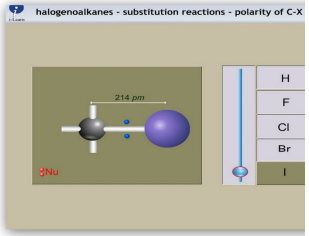


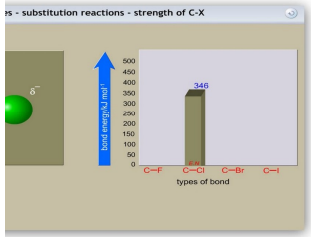


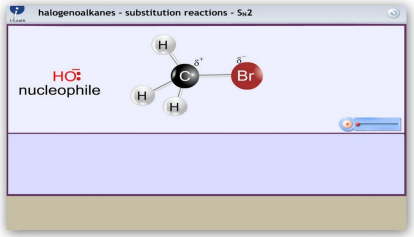


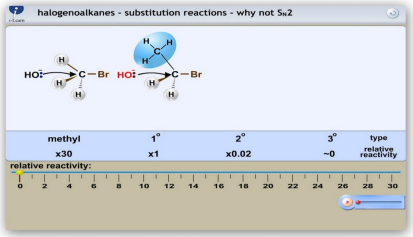


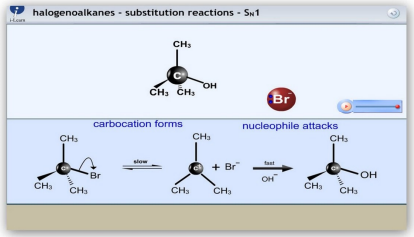
reaction	elimination	substitution
condition	alkene	alcohol
product	heat with reflux	heat with reflux
role of the alkali	tertiary and secondary	primary and secondary
type of halogenoalkanes	acts as a base	acts as a nucleophile
reagent	KOH (aq)	favoured by low temperature
temperature	KOH(ethanol)	favoured by high temperature
concentration of alkali	favoured by high[KOH]	favoured by low[KOH]

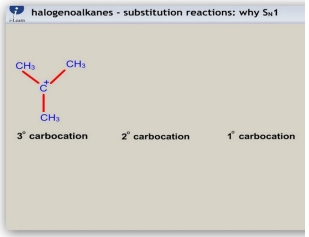


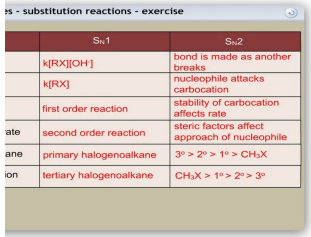




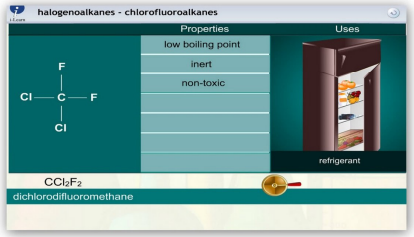


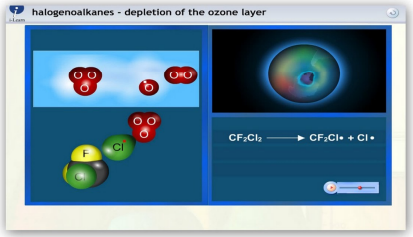


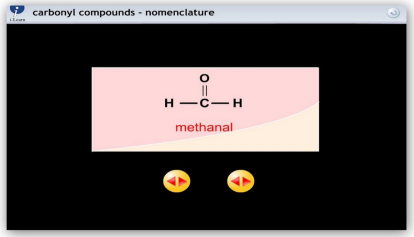


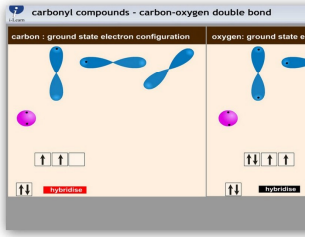


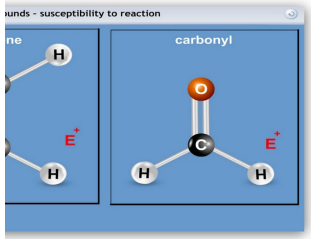
	SN1	SN2
	k[RX][OH⁻]	bond is made as another breaks
	k[RX]	nucleophile attacks carbocation
	first order reaction	stability of carbocation affects rate
ate	second order reaction	steric factors affect approach of nucleophile
ane	primary halogenoalkane	3° > 2° > 1° > CH₃X
ion	tertiary halogenoalkane	CH₃X > 1° > 2° > 3°

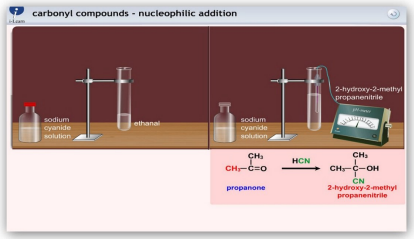


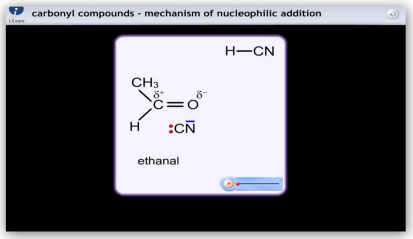


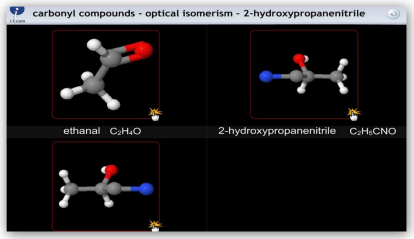


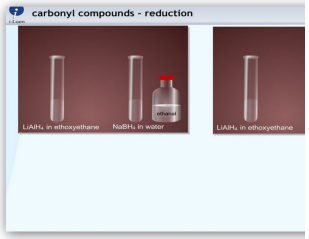


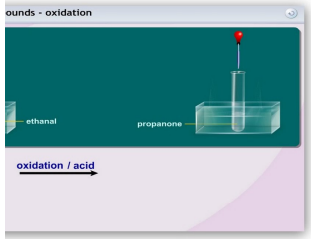


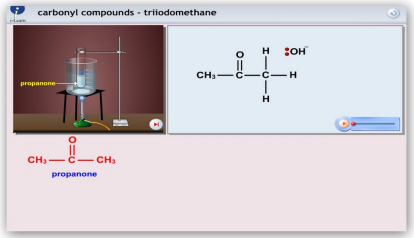


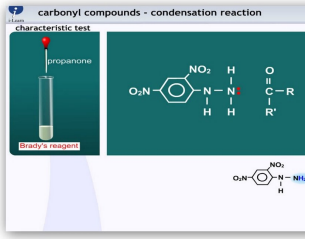


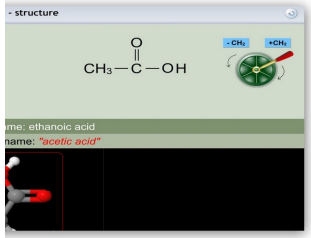


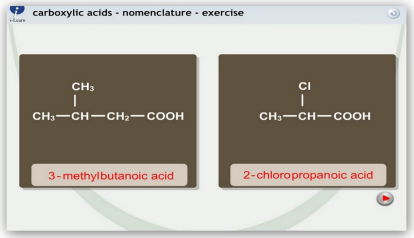


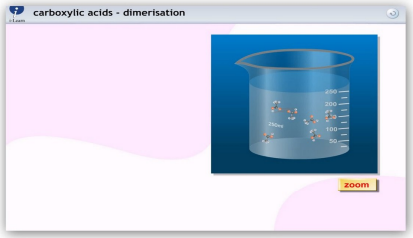


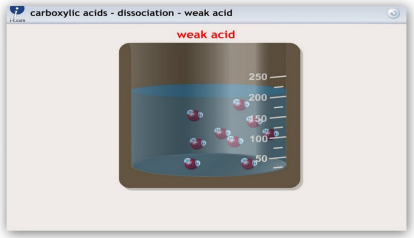


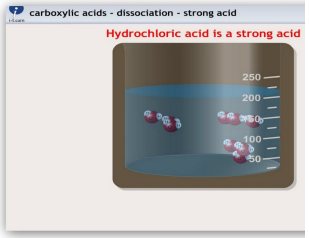


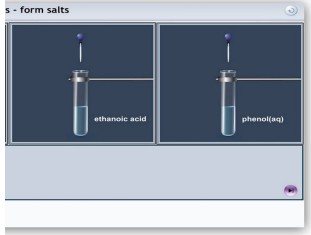

- structure
CH3—C—OH
- CH2
+CH2
me: ethanoic acid
name: "acetic acid"

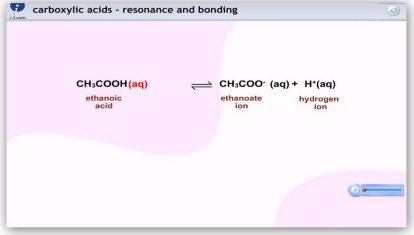

carboxylic acids - nomenclature - exercise
CH3
CH3—CH—CH2—COOH
3-methylbutanoic acid
Cl
CH3—CH—COOH
2-chloropropanoic acid

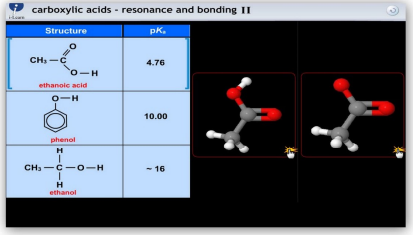

carboxylic acids - dimerisation
zoom

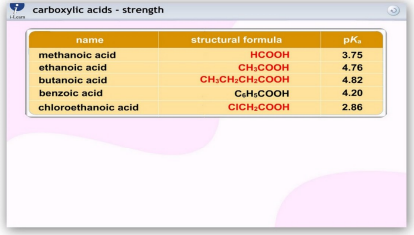

carboxylic acids - dissociation - weak acid
weak acid

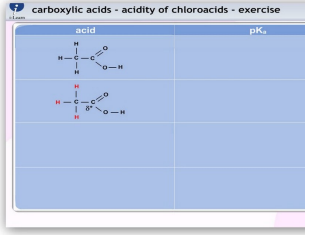

carboxylic acids - dissociation - strong acid
Hydrochloric acid is a strong acid

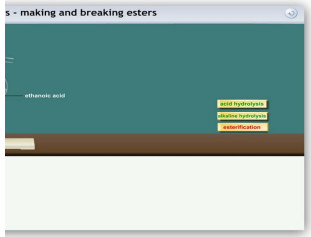

s - form salts
ethanoic acid
phenol(aq)

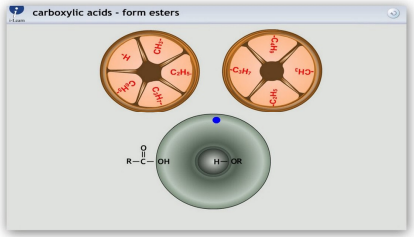

carboxylic acids - resonance and bonding
CH3COOH(aq) ⇌ CH3COO- (aq) + H+(aq)
ethanoic acid
ethanoate ion
hydrogen ion

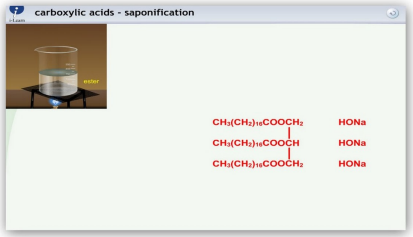

carboxylic acids - resonance and bonding II
Structure
pKa
4.76
ethanoic acid
10.00
phenol
~ 16
ethanol

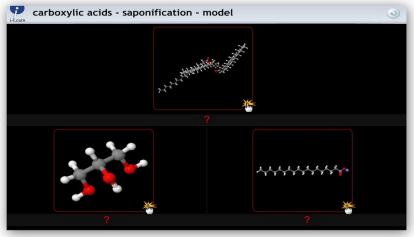

carboxylic acids - strength
name
structural formula
pKa
methanoic acid HCOOH 3.75
ethanoic acid CH3COOH 4.76
butanoic acid CH3CH2CH2COOH 4.82
benzoic acid C6H5COOH 4.20
chloroethanoic acid ClCH2COOH 2.86

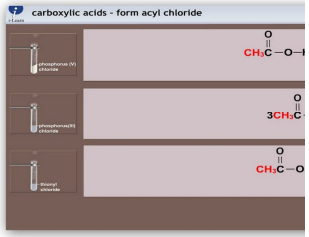

carboxylic acids - acidity of chloroacids - exercise
acid
pKa

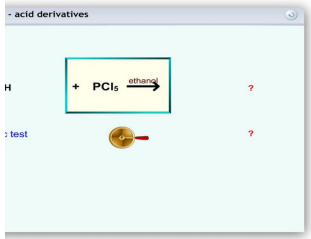

s - making and breaking esters
ethanoic acid
acid hydrolysis
alkaline hydrolysis
esterification

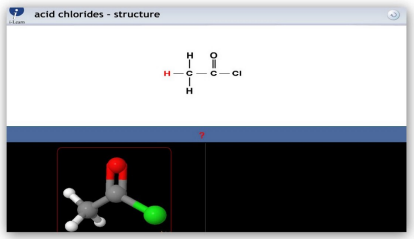

carboxylic acids - form esters

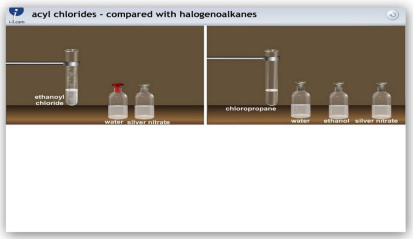

carboxylic acids - saponification
water
CH3(CH2)16COOCH2 HONa
CH3(CH2)16COOCH HONa
CH3(CH2)16COOCH2 HONa

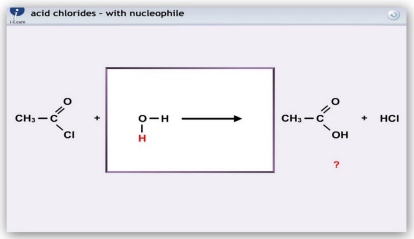

carboxylic acids - saponification - model

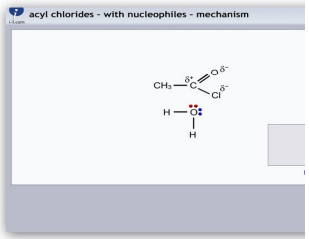

carboxylic acids - form acyl chloride
phosphorus (V) chloride
phosphorus(III) chloride
thionyl chloride

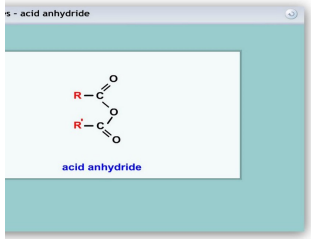

- acid derivatives
+ PCl5
ethanol
test

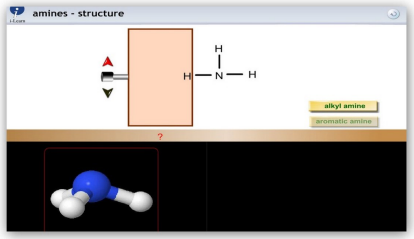

acid chlorides - structure

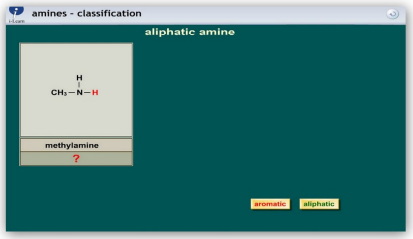

acyl chlorides - compared with halogenoalkanes
ethanoyl chloride
water
silver nitrate
chloropropane
ethanol

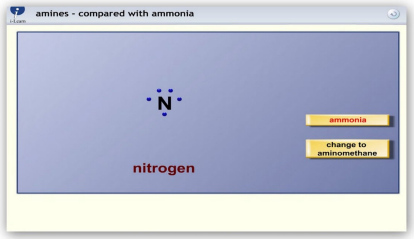

acid chlorides - with nucleophile
CH3—C—Cl
O—H
H
CH3—C—OH
+ HCl

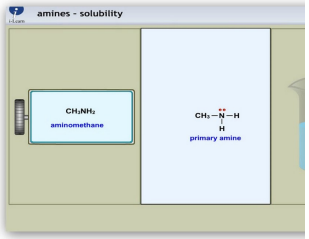

acyl chlorides - with nucleophiles - mechanism

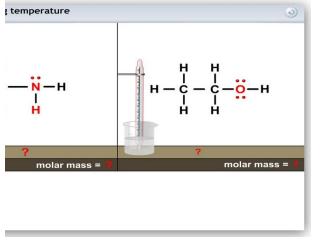

s - acid anhydride
R—C—O—C—R'
acid anhydride

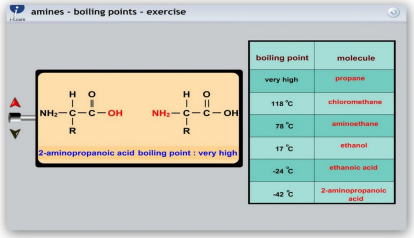

amines - structure
H—N—H
alkyl amine
aromatic amine

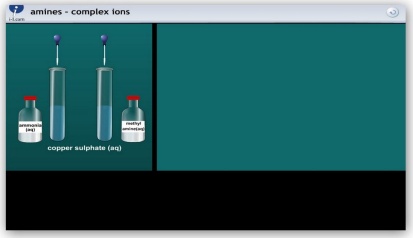

amines - classification
aliphatic amine
CH3—N—H
methylamine
aromatic
aliphatic

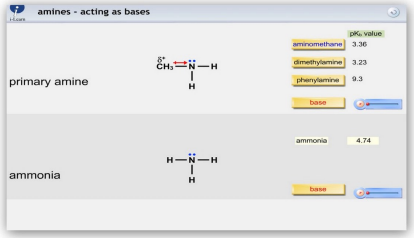

amines - compared with ammonia
N
nitrogen
ammonia
change to aminomethane

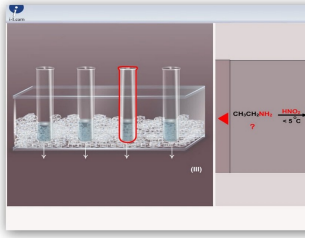

amines - solubility
CH3NH2
aminomethane
primary amine

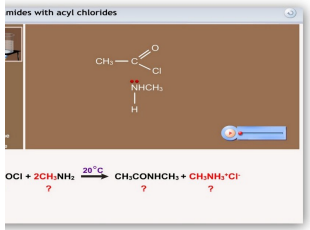

temperature
molar mass =
molar mass =

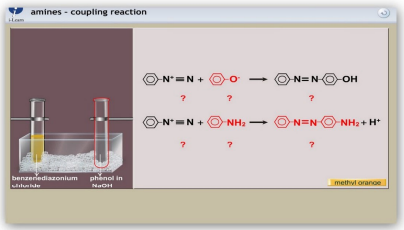

amines - boiling points - exercise
2-aminopropanoic acid boiling point : very high
boiling point
molecule
very high propane
118 °C chloromethane
78 °C aminoethane
17 °C ethanol
-24 °C ethanoic acid
-42 °C 2-aminopropanoic acid

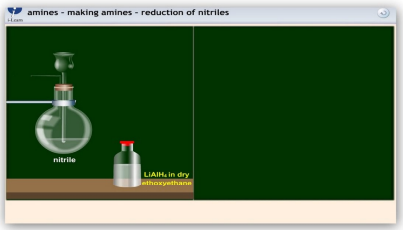

amines - complex ions
copper sulphate (aq)

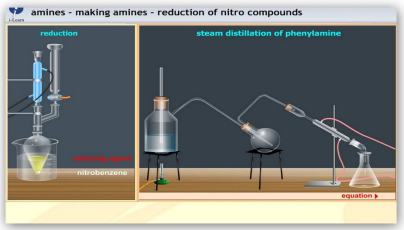

amines - acting as bases
pKb value
primary amine
aminomethane 3.36
dimethylamine 3.23
phenylamine 9.3
base
ammonia
ammonia 4.74
base

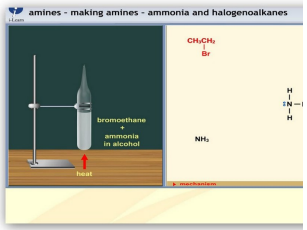

(III)

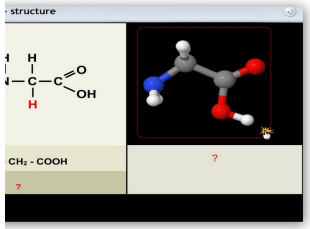

mides with acyl chlorides
20°C

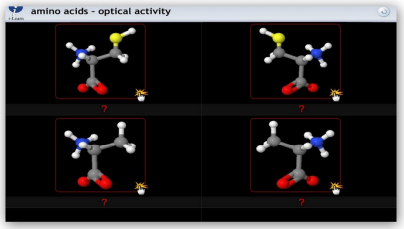

amines - coupling reaction
benzenediazonium chloride
phenol in NaOH
methyl orange

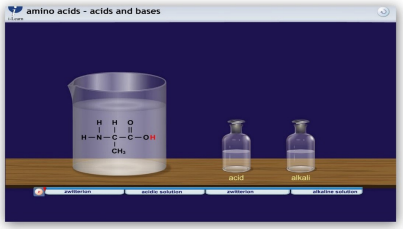

amines - making amines - reduction of nitriles
nitrile
LiAlH₄ in dry ethoxyethane

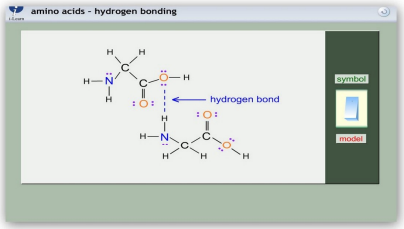

amines - making amines - reduction of nitro compounds
reduction
steam distillation of phenylamine
nitrobenzene
equation

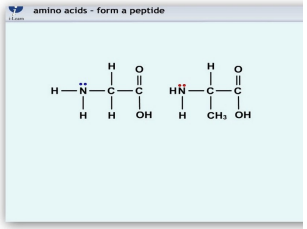

amines - making amines - ammonia and halogenoalkanes
bromoethane + ammonia in alcohol
heat

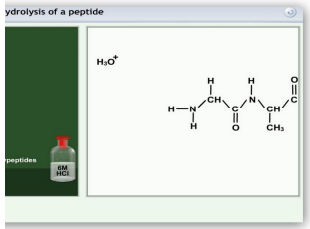

structure

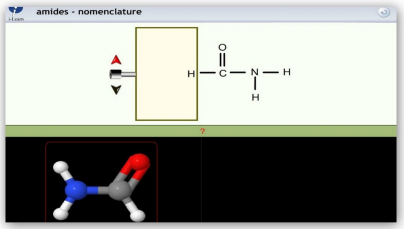

amino acids - optical activity

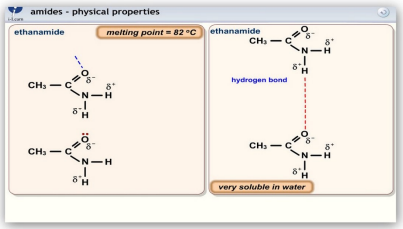

amino acids - acids and bases
acid
alkali

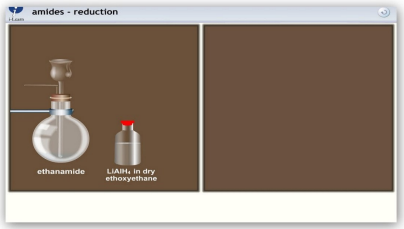

amino acids - hydrogen bonding
hydrogen bond
symbol
model

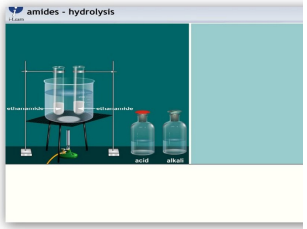

amino acids - form a peptide

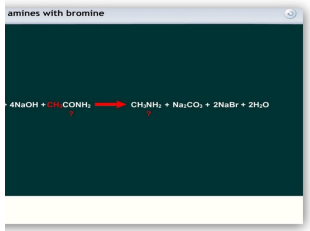

ydrolysis of a peptide

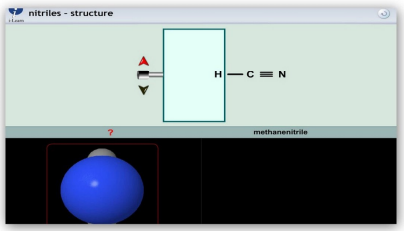

amides - nomenclature

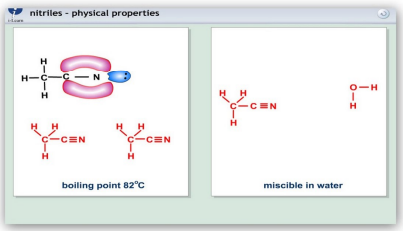

amides - physical properties
ethanamide
melting point = 82 °C
hydrogen bond
very soluble in water

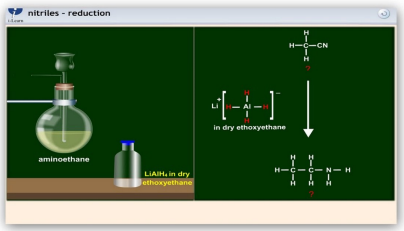

amides - reduction
ethanamide
LiAlH₄ in dry ethoxyethane

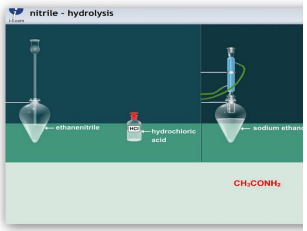

amides - hydrolysis
acid
alkali

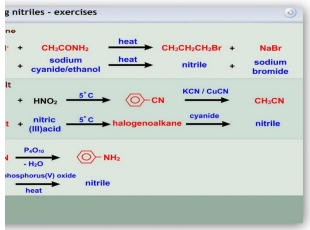

amines with bromine

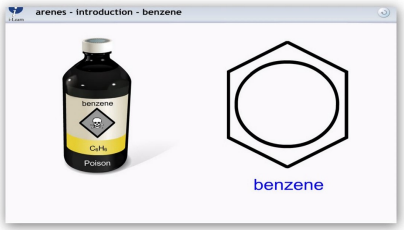

nitriles - structure
methanenitrile

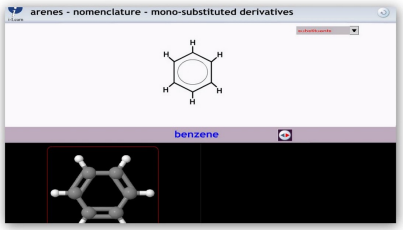

nitriles - physical properties
boiling point 82°C
miscible in water

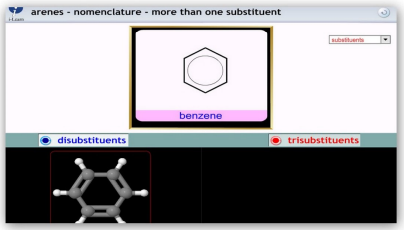

nitriles - reduction
aminoethane
LiAlH₄ in dry ethoxyethane
in dry ethoxyethane

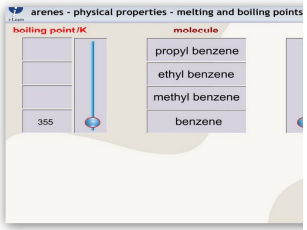

nitrile - hydrolysis
ethanenitrile
hydrochloric acid
CH₃CONH₂

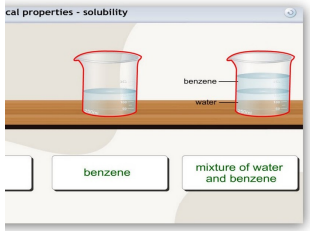

g nitriles - exercises
heat
sodium cyanide/ethanol
nitrile
sodium bromide
5°C
KCN / CuCN
cyanide
halogenoalkane
nitrile

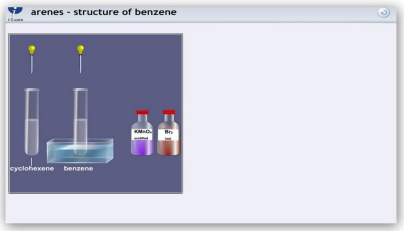

arenes - introduction - benzene
benzene
Poison
benzene

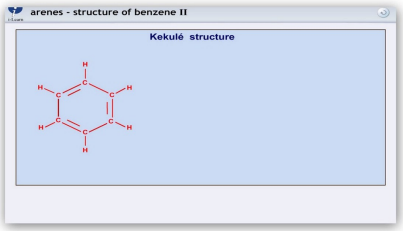

arenes - nomenclature - mono-substituted derivatives
benzene

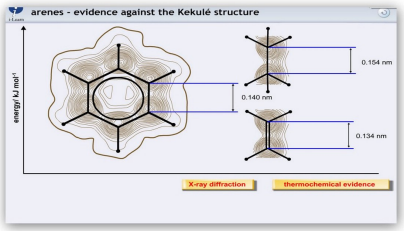

arenes - nomenclature - more than one substituent
benzene
disubstituents
trisubstituents

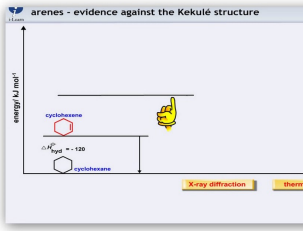

arenes - physical properties - melting and boiling points
boiling point/K
molecule
propyl benzene
ethyl benzene
methyl benzene
benzene
355

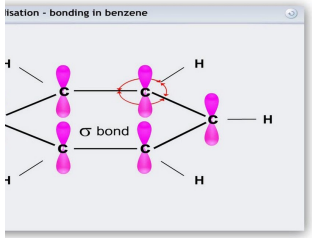

cal properties - solubility
benzene
water
benzene
mixture of water and benzene

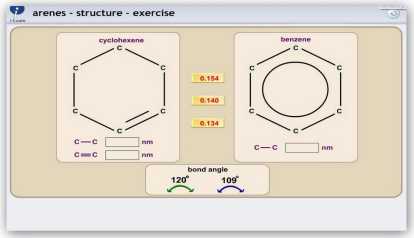

arenes - structure of benzene
cyclohexene
benzene

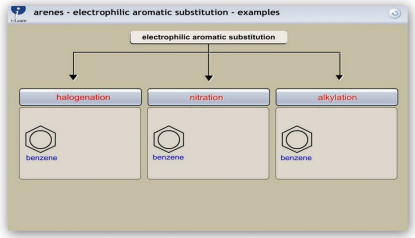

arenes - structure of benzene II
Kekulé structure

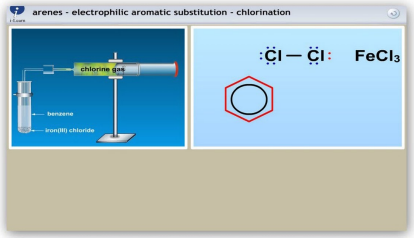

arenes - evidence against the Kekulé structure
energy/ kJ mol⁻¹
0.154 nm
0.140 nm
0.134 nm
X-ray diffraction
thermochemical evidence

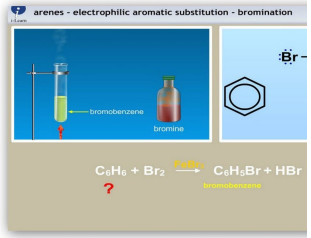

arenes - evidence against the Kekulé structure
energy/ kJ mol⁻¹
cyclohexene
cyclohexane
X-ray diffraction

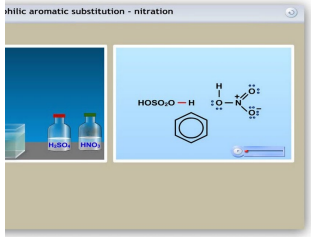


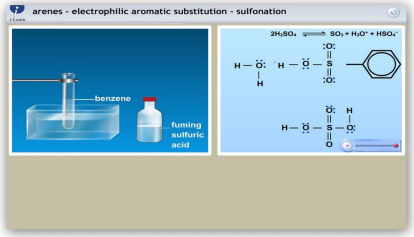


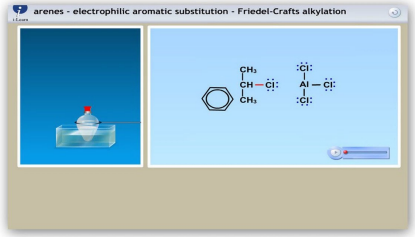


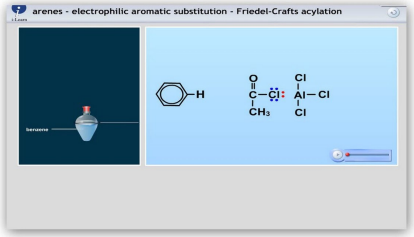


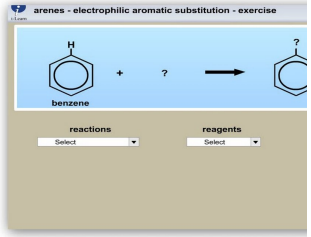


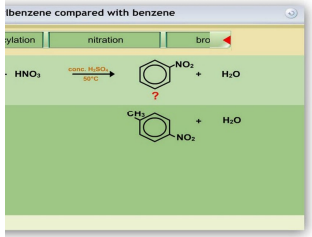


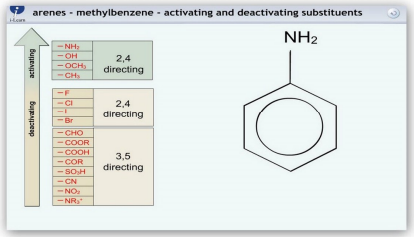


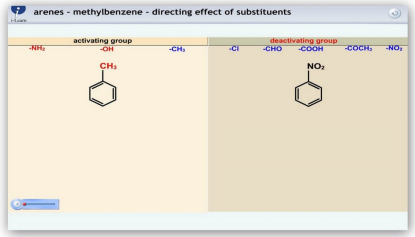


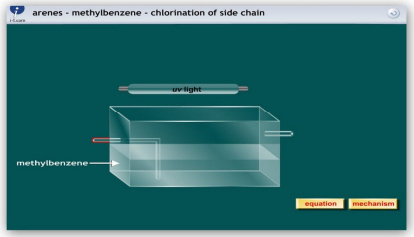


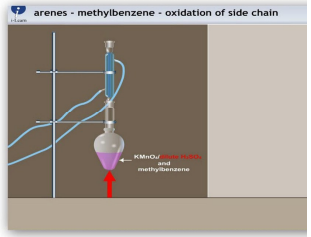


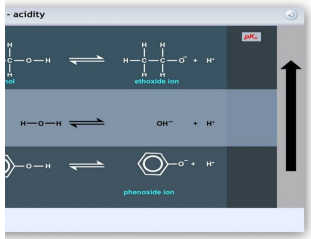


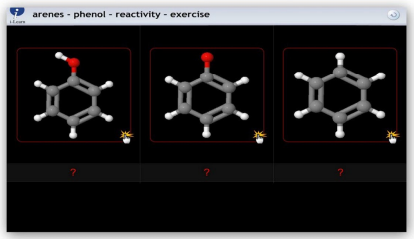




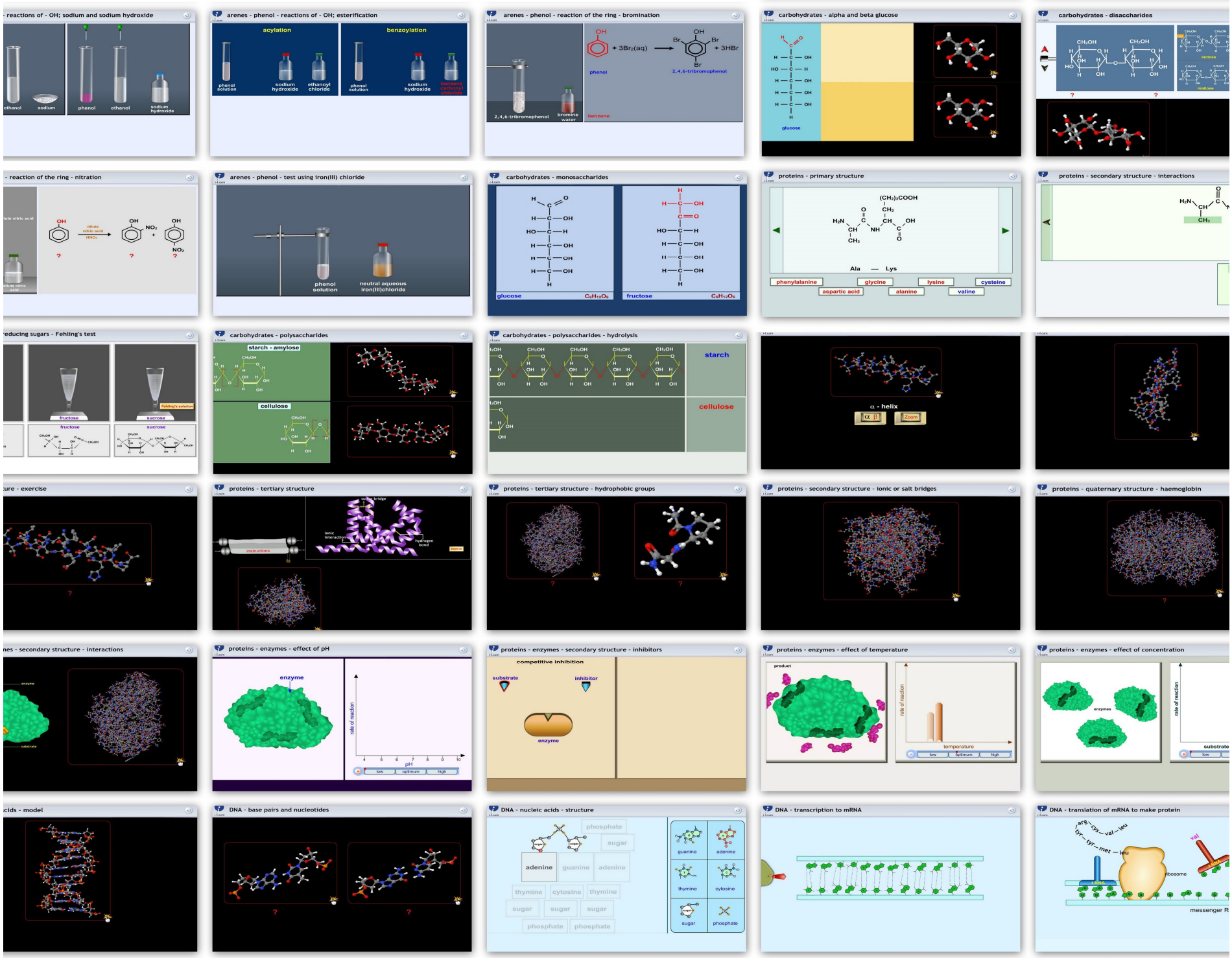








protein, carbs...


reactions of - OH; sodium and sodium hydroxide
ethanol
sodium
phenol
ethanol
sodium hydroxide
arenes - phenol - reactions of - OH; esterification
acylation
benzoylation
phenol solution
sodium hydroxide
ethanoyl chloride
phenol solution
sodium hydroxide
benzene carbonyl chloride
arenes - phenol - reaction of the ring - bromination
2,4,6-tribromophenol
bromine water
phenol
2,4,6-tribromophenol
benzene
carbohydrates - alpha and beta glucose
glucose
carbohydrates - disaccharides
lactose
maltose
reaction of the ring - nitration
dilute nitric acid
arenes - phenol - test using iron(III) chloride
phenol solution
neutral aqueous iron(III)chloride
carbohydrates - monosaccharides
glucose
fructose
proteins - primary structure
Ala — Lys
phenylalanine
glycine
lysine
cysteine
aspartic acid
alanine
valine
proteins - secondary structure - interactions
reducing sugars - Fehling's test
fructose
sucrose
Fehling's solution
carbohydrates - polysaccharides
starch - amylose
cellulose
carbohydrates - polysaccharides - hydrolysis
starch
cellulose
α - helix
Zoom
exercise
proteins - tertiary structure
proteins - tertiary structure - hydrophobic groups
proteins - secondary structure - ionic or salt bridges
proteins - quaternary structure - haemoglobin
secondary structure - interactions
proteins - enzymes - effect of pH
enzyme
rate of reaction
pH
low
optimum
high
proteins - enzymes - secondary structure - inhibitors
competitive inhibition
substrate
inhibitor
enzyme
proteins - enzymes - effect of temperature
product
rate of reaction
temperature
low
optimum
high
proteins - enzymes - effect of concentration
enzymes
rate of reaction
substrate
low
acids - model
DNA - base pairs and nucleotides
DNA - nucleic acids - structure
phosphate
sugar
adenine
guanine
adenine
thymine
cytosine
thymine
sugar
sugar
sugar
phosphate
phosphate
guanine
adenine
thymine
cytosine
sugar
phosphate
DNA - transcription to mRNA
DNA - translation of mRNA to make protein
arg
cys
val
leu
tyr
tyr
met
leu
val
ribosome
tRNA
messenger R