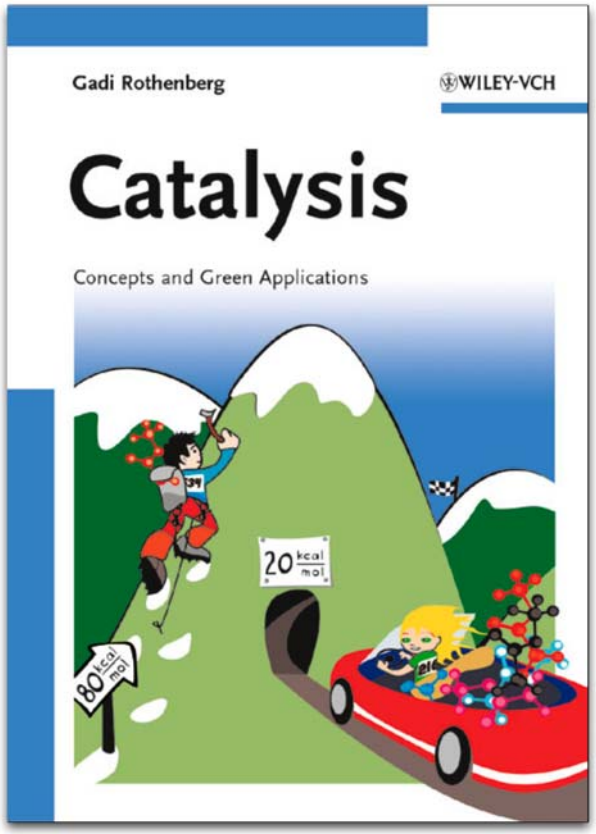
Catalysis: Concepts and Green Applications

Lecture slides for Chapter 1: Introduction to catalysis, green chemistry, and sustainable development.

Most of the graphics here were drawn using PowerPoint and Chemdraw (version Ultra 9.0).

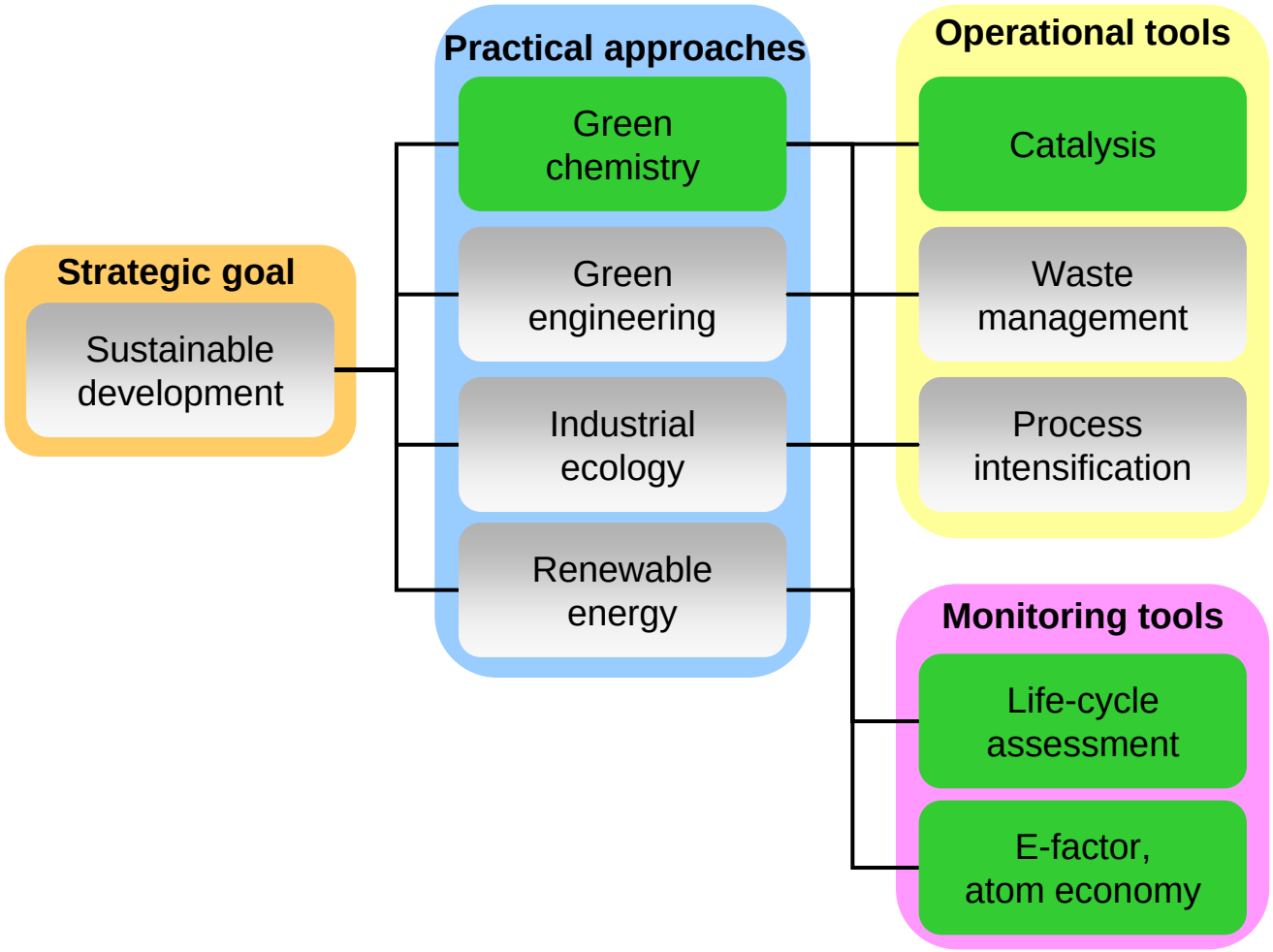
Feel free to modify and/or add your own pyrotechnics.

Please send any feedback to feedback@catalysisbook.org

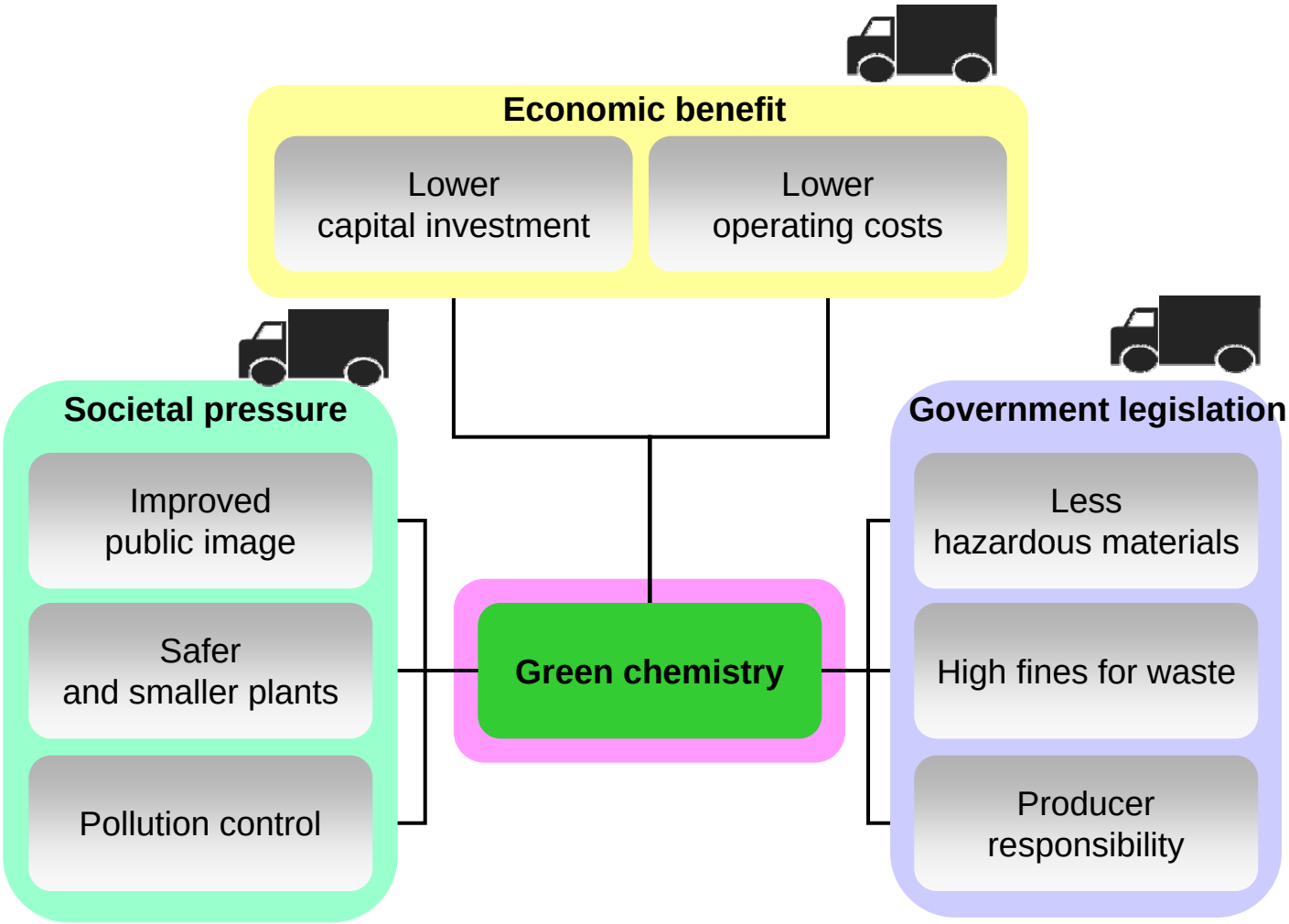


Catalysis/ Rothenberg, ISBN 978-3-527-31824-7.

The big picture

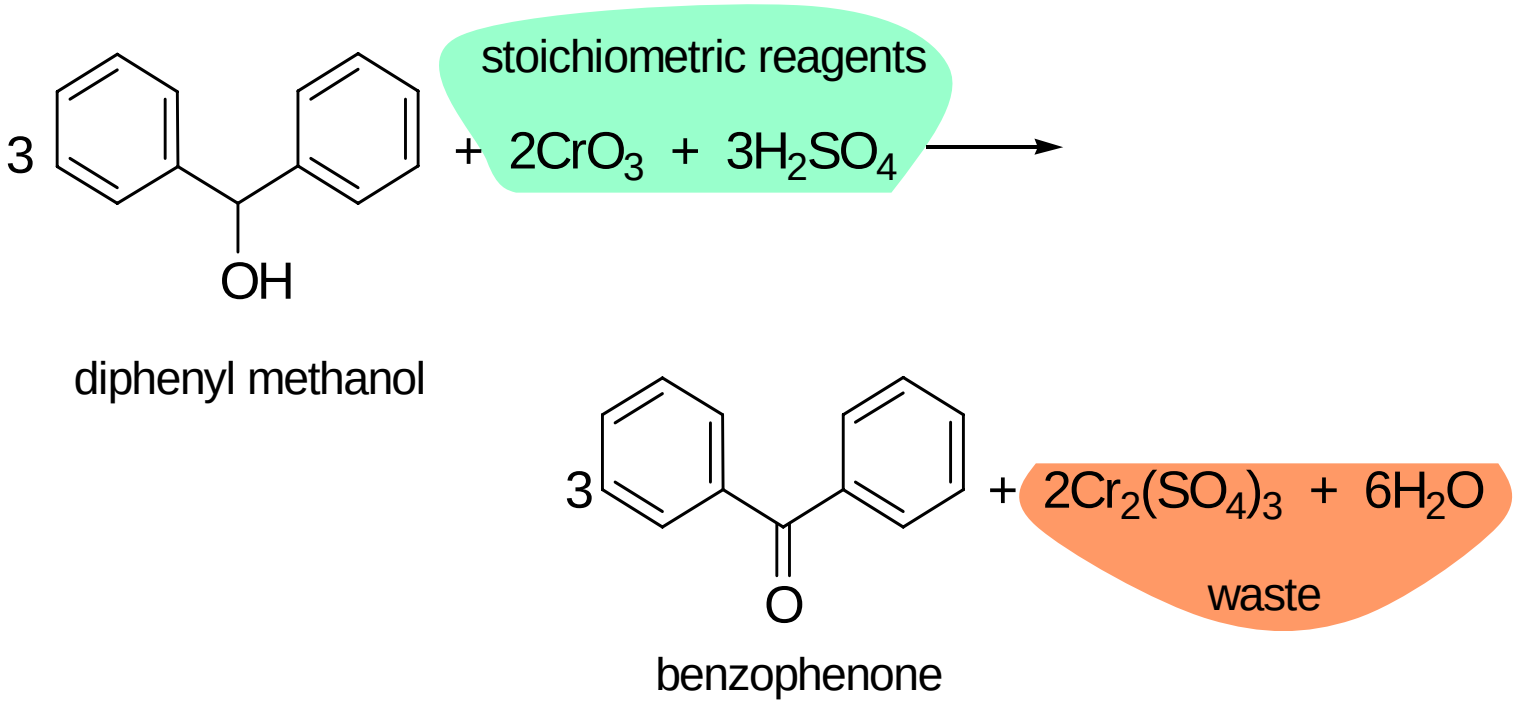


The drivers of green chemistry

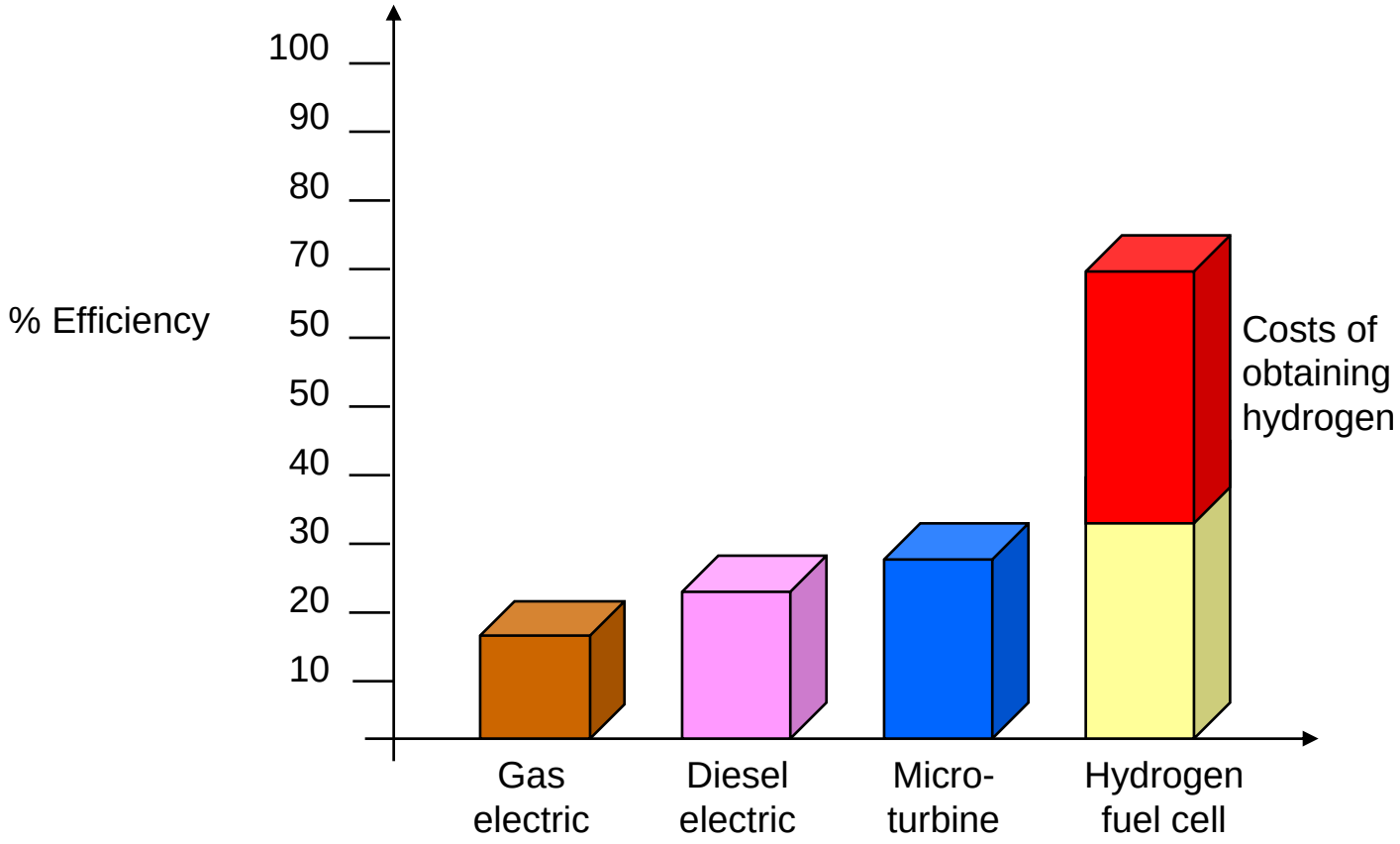


Catalysis/ Rothenberg, ISBN 978-3-527-31824-7.

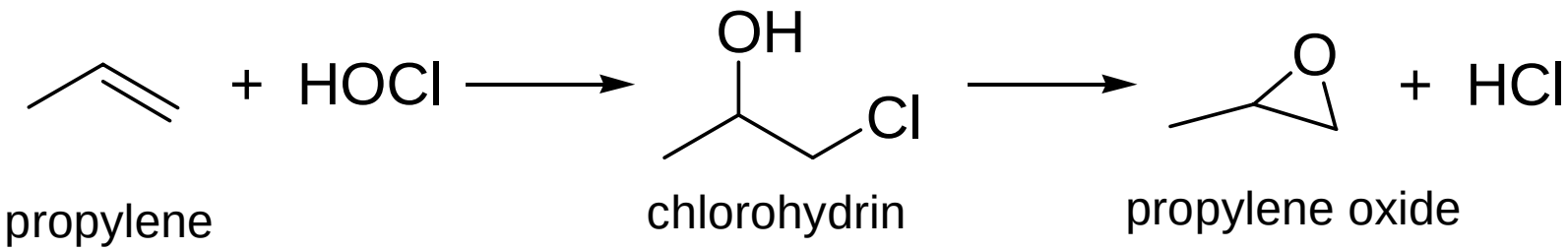
Oxidation of diphenylmethanol to benzophenone

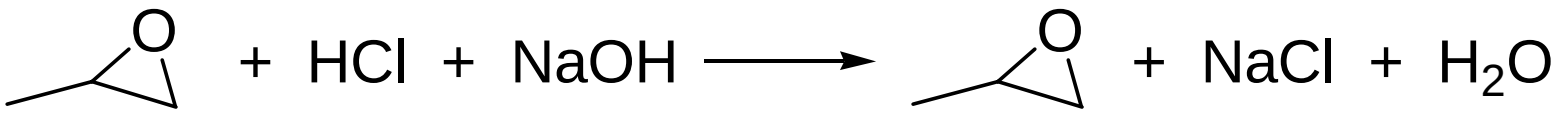


Relative efficiency of various engine types

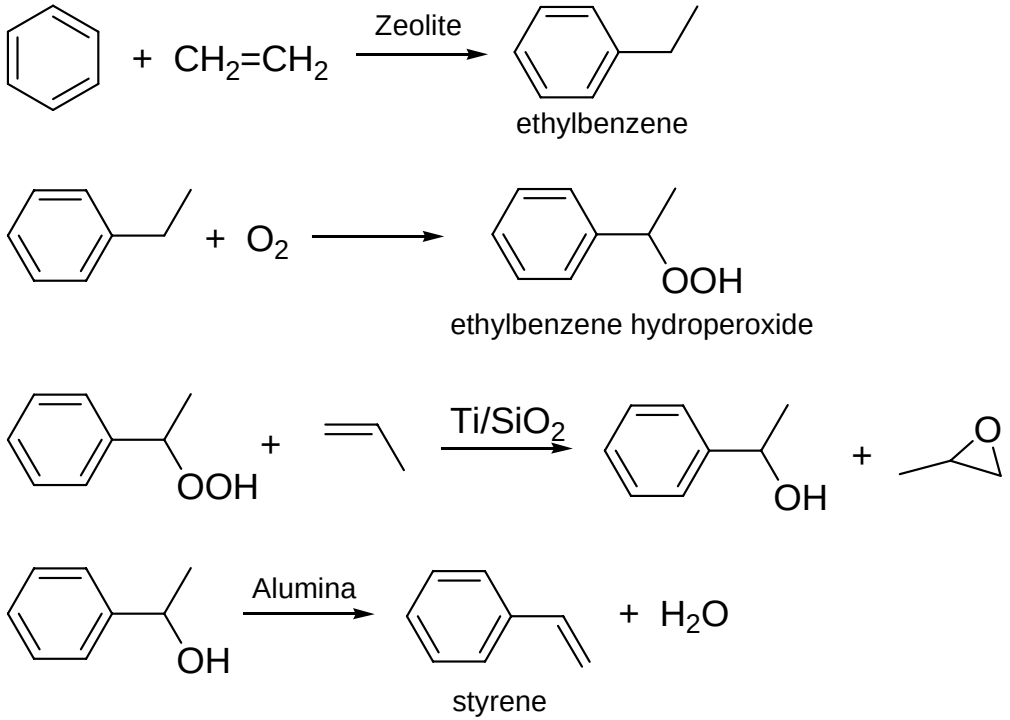


The traditional propene oxide route

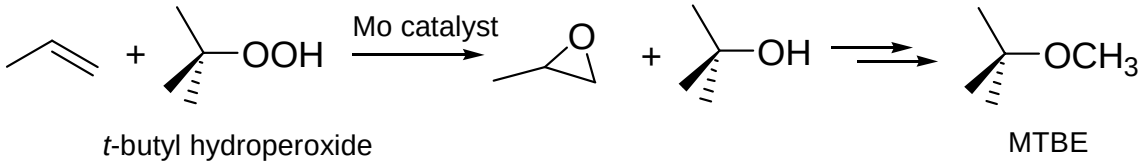




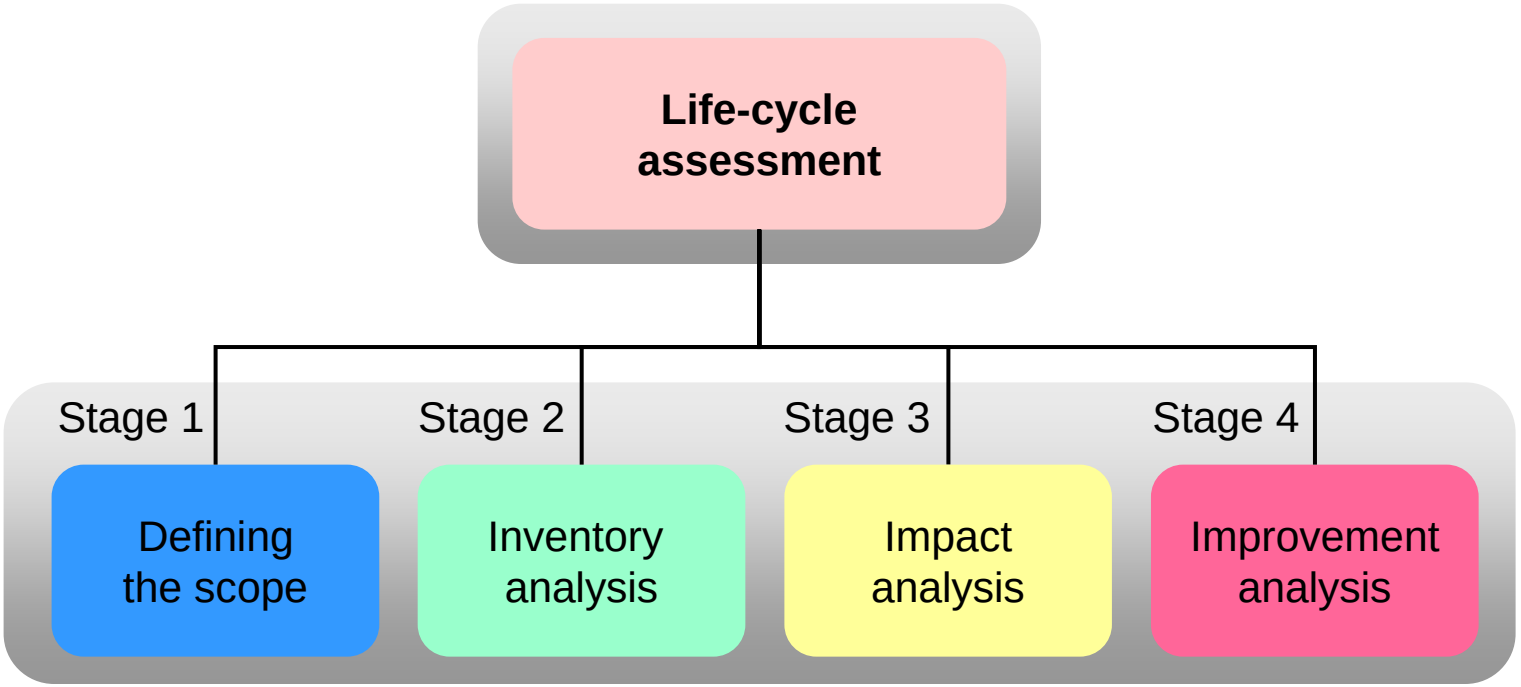
The SMPO process



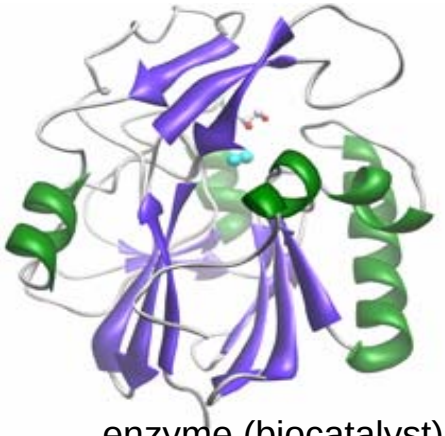
Catalytic oxidation of propene



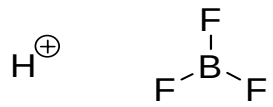
The four stages of life-cycle assessment



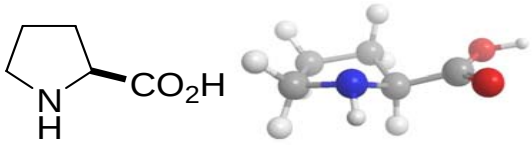
Different types of catalysts



enzyme (biocatalyst)

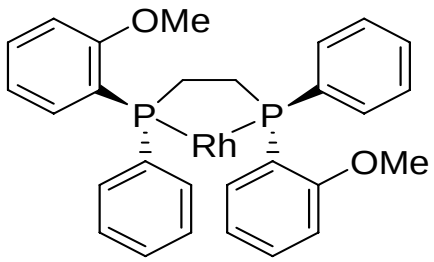


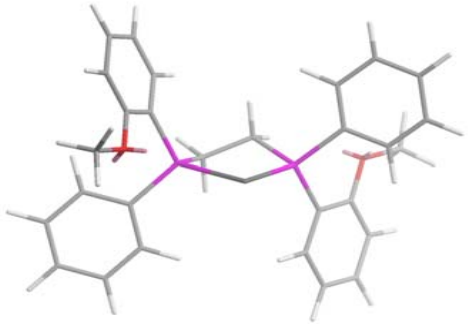
homogeneous acid catalysts



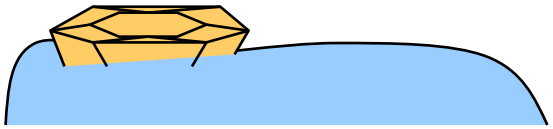
L-proline (organocatalyst)

zeolite (crystalline aluminosilicate)





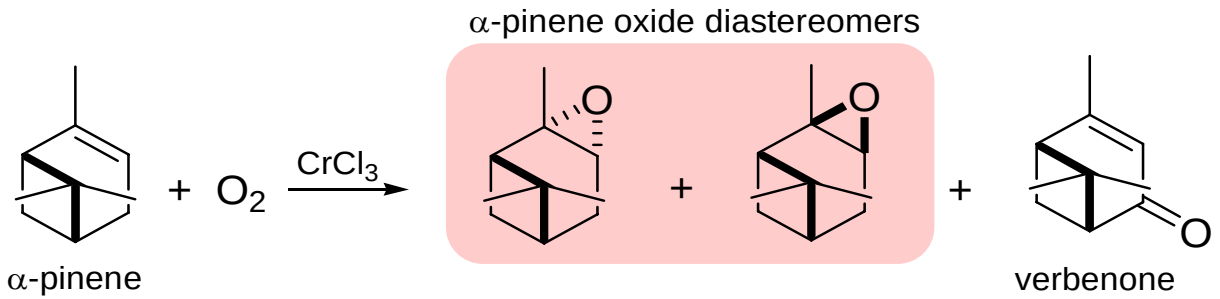
(*R*,*R*)-DiPAMP-Rh (organometallic complex)



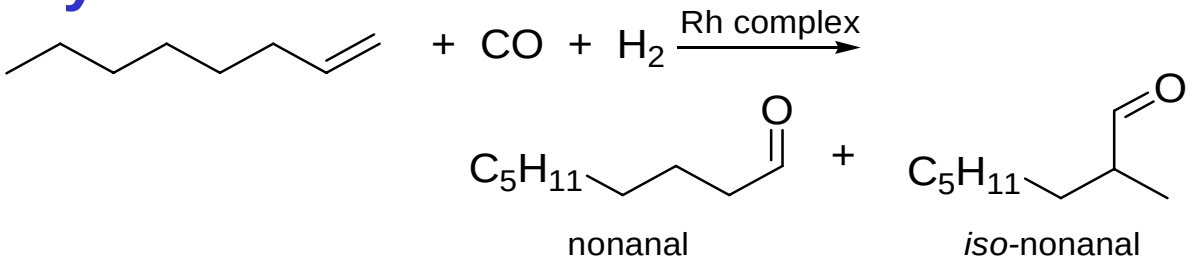
copper-zinc crystallites on silica

Catalysis/ Rothenberg, ISBN 978-3-527-31824-7.

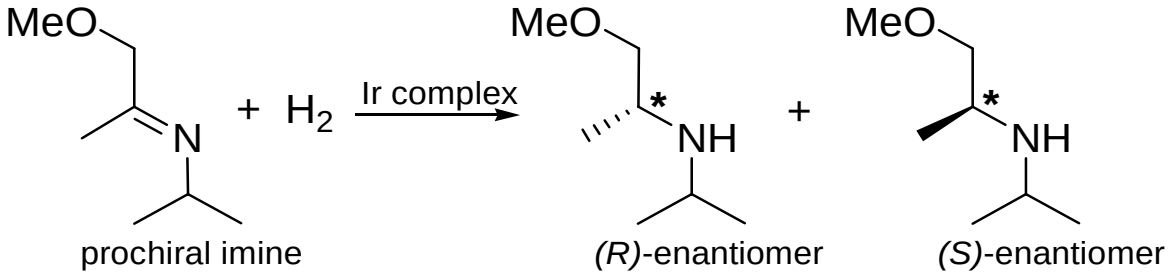
Examples of chemo- and diastereoselectivity



Regioselectivity

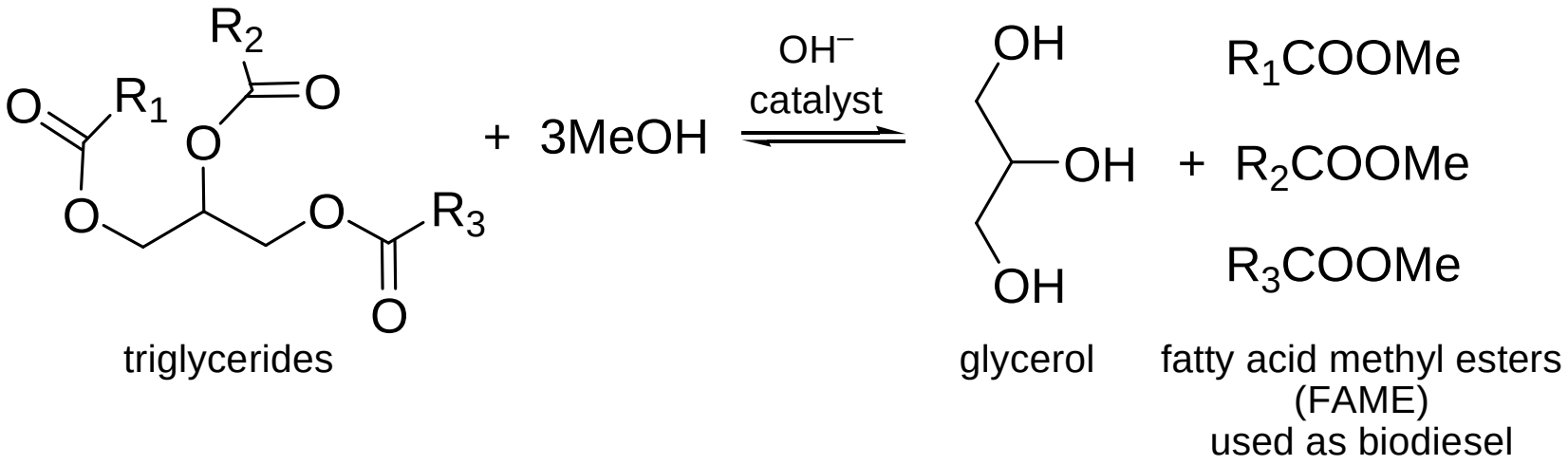


Enantioselectivity



Catalysis/ Rothenberg, ISBN 978-3-527-31824-7.

Base-catalysed transesterification of triglycerides



triglycerides

glycerol

fatty acid methyl esters (FAME) used as biodiesel

Figure 1.11

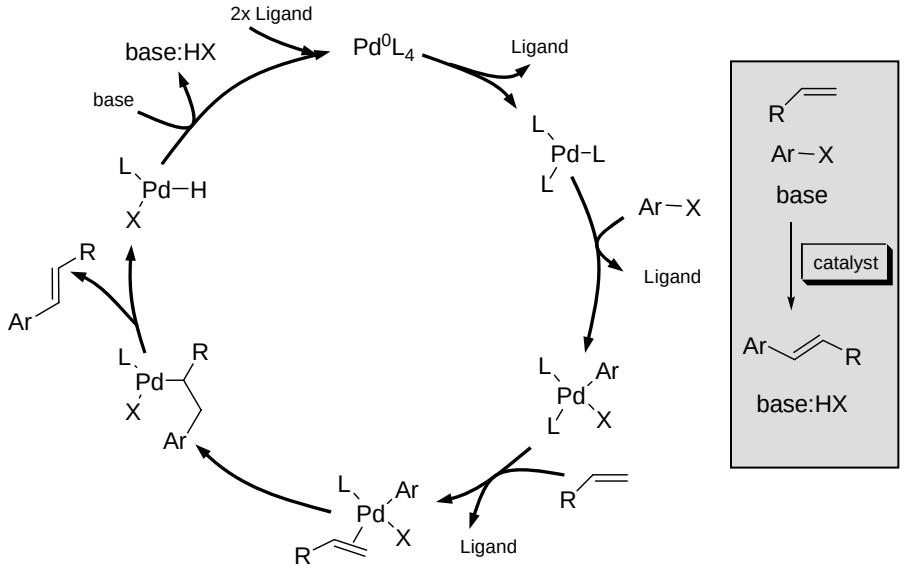

2x Ligand
base:HX
base
Pd0L4
Ligand
L
Pd−L
L
Ar−X
Ligand
L
Pd
Ar
L
X
R
Ar
L
Pd
X
R
Ar
L
Pd
Ar
X
R
Ligand
R
L
Pd−H
X
R
Ar−X
base
catalyst
Ar
R
base:HX

Figure 1.12

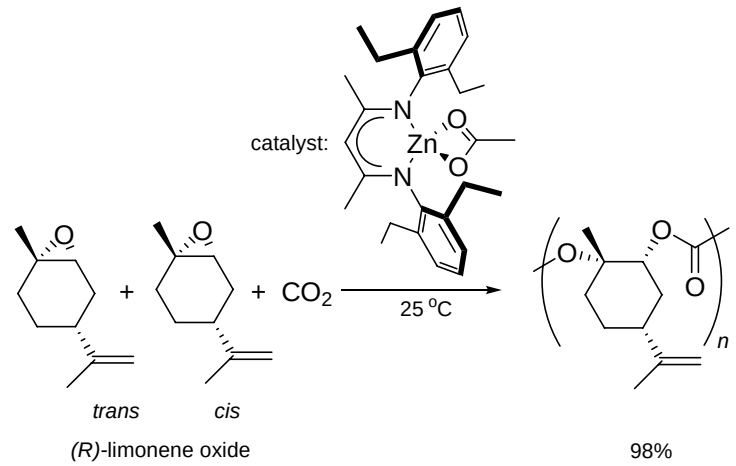

catalyst:
N
Zn
O
O
N
O
O
+
+ CO2
25 °C
O
O
O
n
trans
cis
(R)-limonene oxide
98%

Figure 1.13

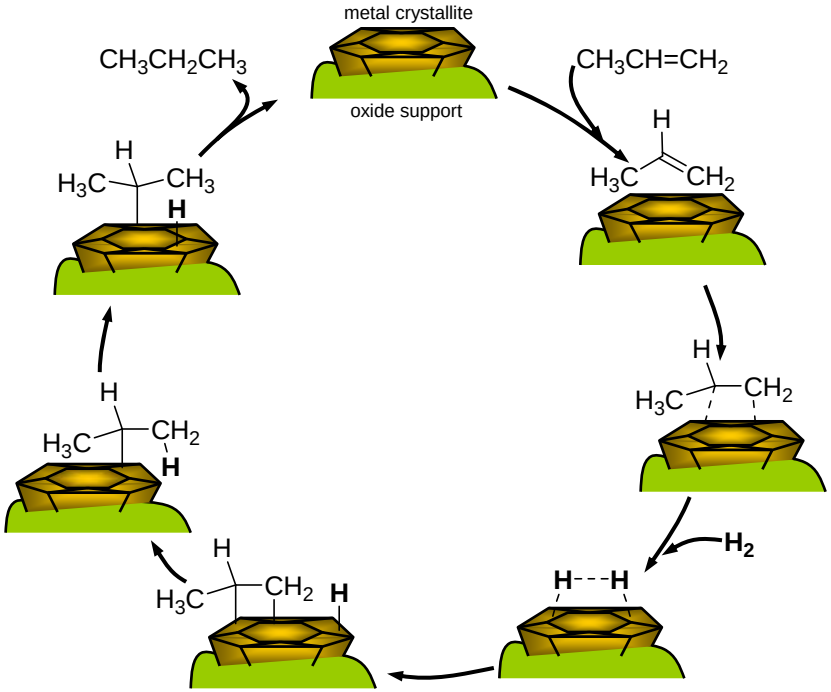


Figure 1.14

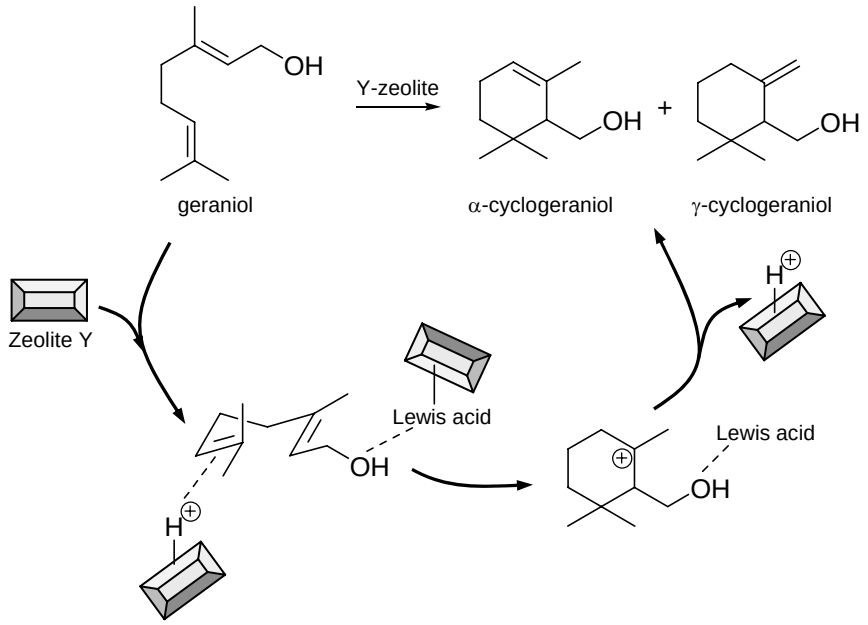

OH
Y-zeolite
OH
+
OH
geraniol
α-cyclogeraniol
γ-cyclogeraniol
Zeolite Y
Lewis acid
OH
H
Lewis acid
OH
H

Figure 1.15

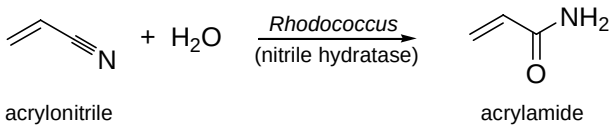

+ H_2O
Rhodococcus
(nitrile hydratase)
NH_2
O
N
acrylonitrile
acrylamide

Figure 1.16

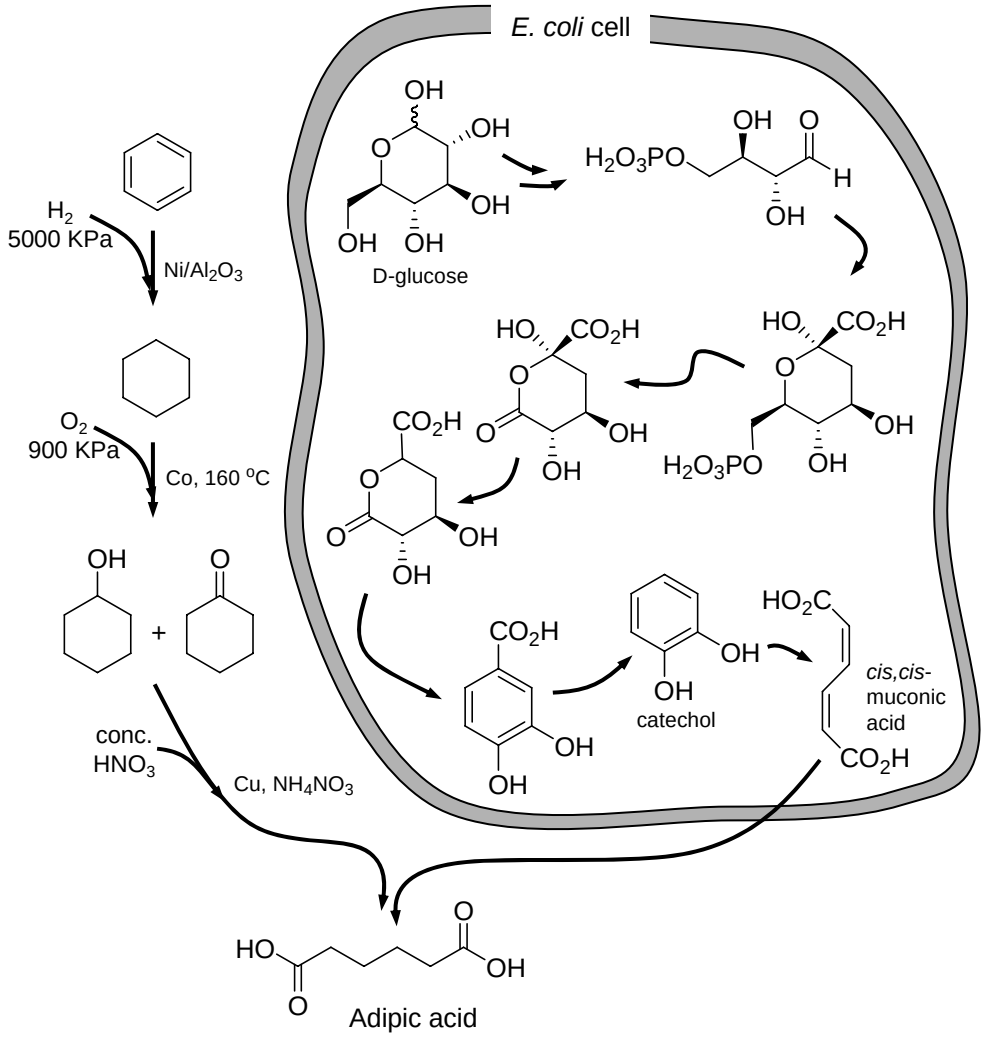

E. coli cell
D-glucose
H2
5000 KPa
Ni/Al2O3
O2
900 KPa
Co, 160 °C
conc.
HNO3
Cu, NH4NO3
catechol
cis,cis-
muconic
acid
Adipic acid

Figure 1.17

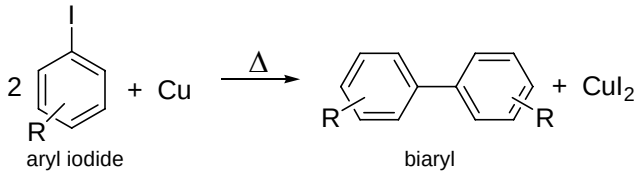


Figure 1.18

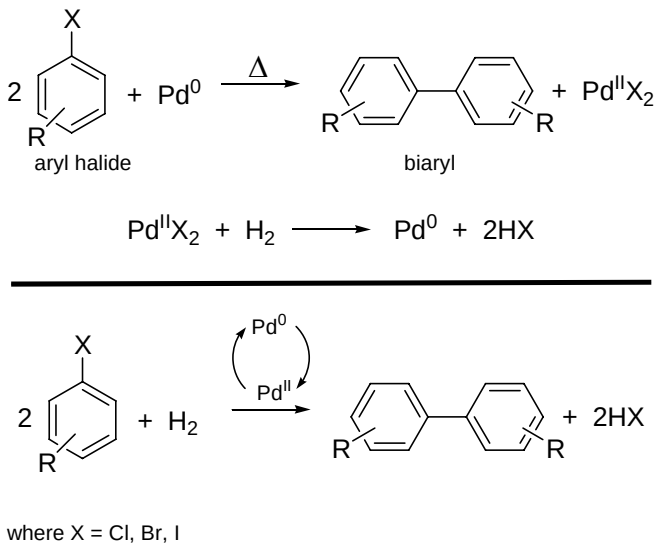

X
2
+ Pd0
Δ
R
aryl halide
biaryl
+ PdIIX2
PdIIX2 + H2
Pd0 + 2HX
Pd0
PdII
+ H2
+ 2HX
where X = Cl, Br, I

Figure 1.19

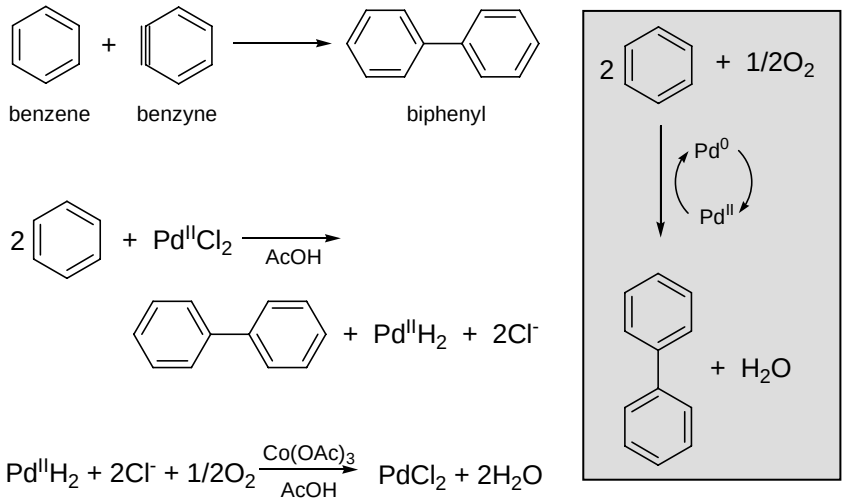

benzene
benzyne
biphenyl
2
+ Pd^II Cl2
AcOH
+ Pd^II H2 + 2Cl-
Pd^II H2 + 2Cl- + 1/2O2
Co(OAc)3
AcOH
PdCl2 + 2H2O
2
+ 1/2O2
Pd0
PdII
+ H2O

Figure 1.20

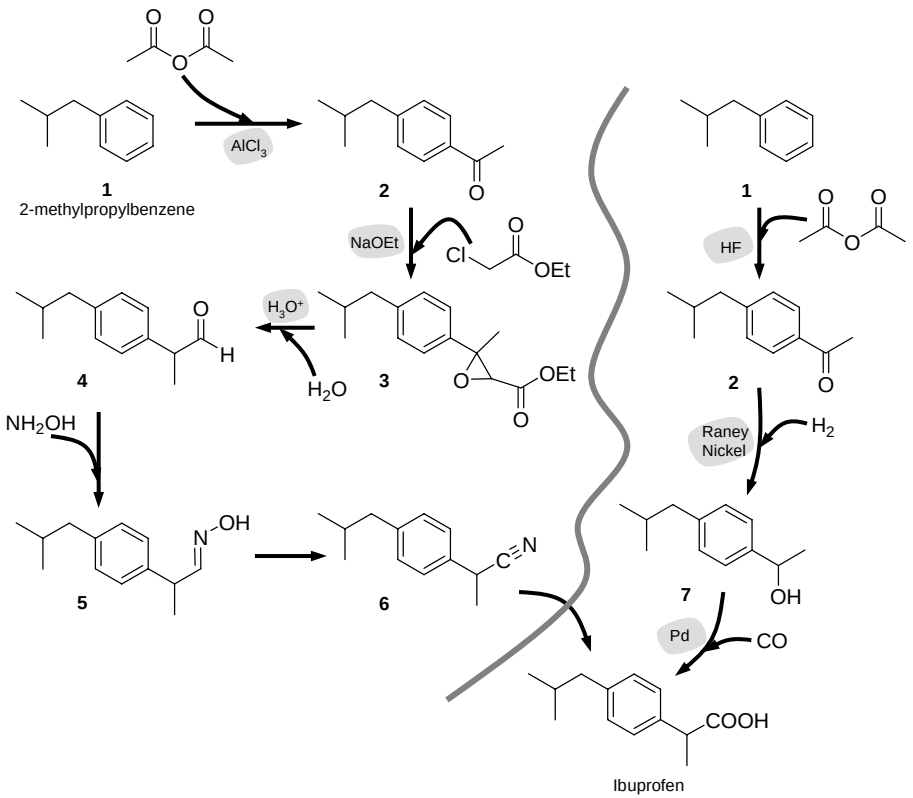

1
2-methylpropylbenzene
AlCl3
2
NaOEt
Cl
OEt
3
H3O+
H2O
4
NH2OH
5
N-OH
6
C≡N
1
HF
2
Raney Nickel
H2
7
OH
Pd
CO
COOH
Ibuprofen

Figure 1.21

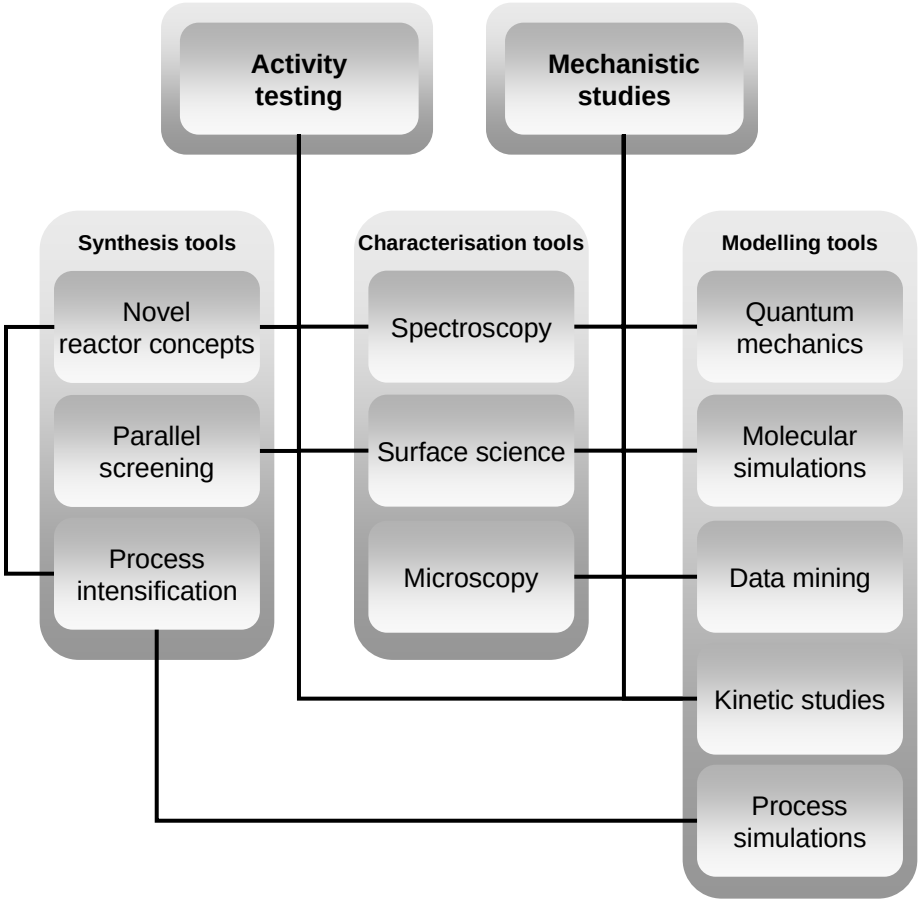

Activity testing
Mechanistic studies
Synthesis tools
Novel reactor concepts
Parallel screening
Process intensification
Characterisation tools
Spectroscopy
Surface science
Microscopy
Modelling tools
Quantum mechanics
Molecular simulations
Data mining
Kinetic studies
Process simulations

Figure 1.22

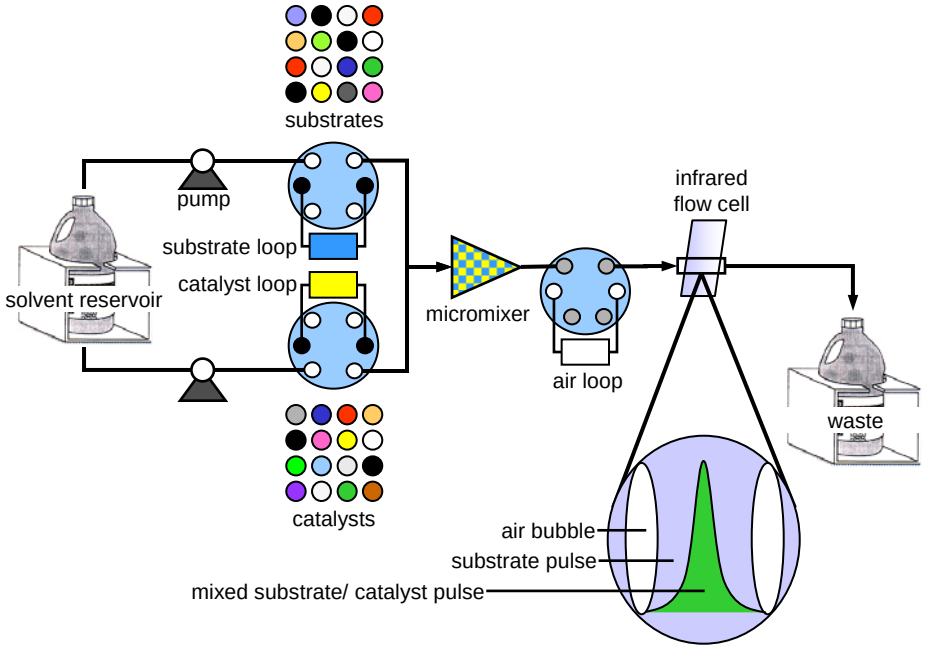

substrates
pump
substrate loop
catalyst loop
solvent reservoir
micromixer
air loop
infrared
flow cell
waste
catalysts
air bubble
substrate pulse
mixed substrate/ catalyst pulse

Figure 1.23

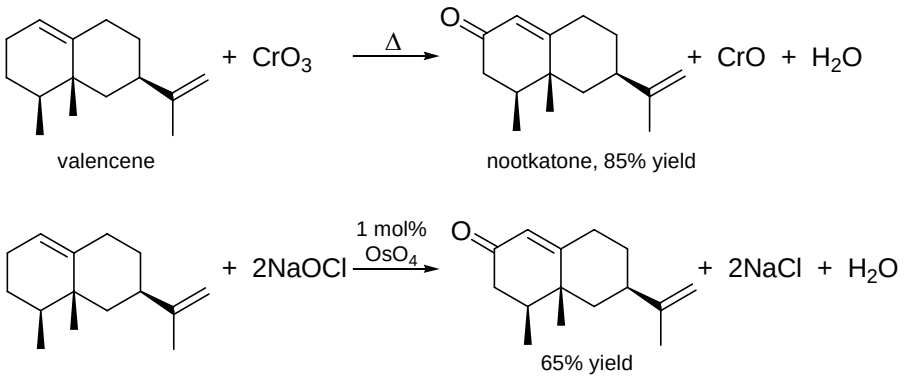

+ CrO_3
Δ
O
+ CrO + H_2O
valencene
nootkatone, 85% yield
+ 2NaOCl
1 mol%
OsO_4
O
+ 2NaCl + H_2O
65% yield

Figure 1.24

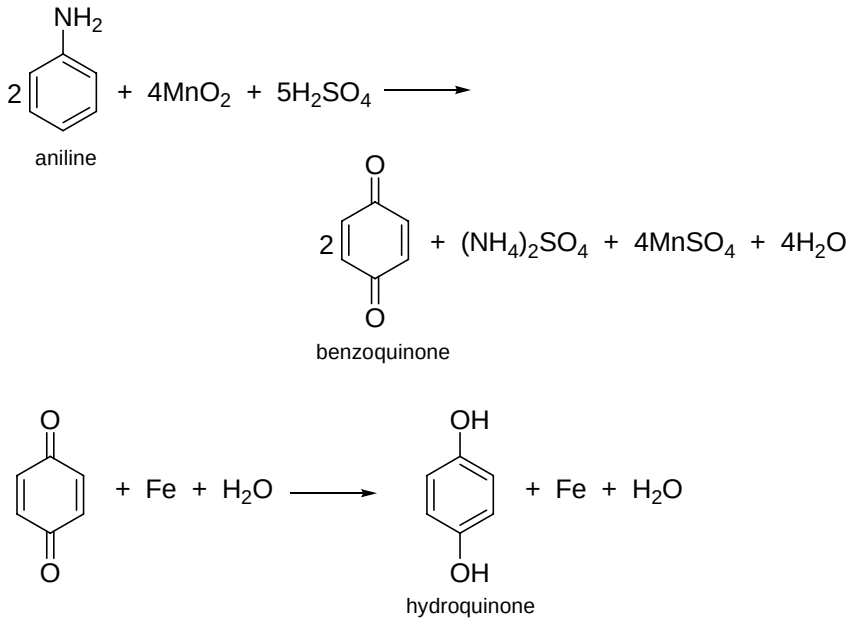

NH2
2
+ 4MnO2 + 5H2SO4
aniline
O
2
+ (NH4)2SO4 + 4MnSO4 + 4H2O
O
benzoquinone
O
+ Fe + H2O
O
OH
+ Fe + H2O
OH
hydroquinone

Figure 1.25

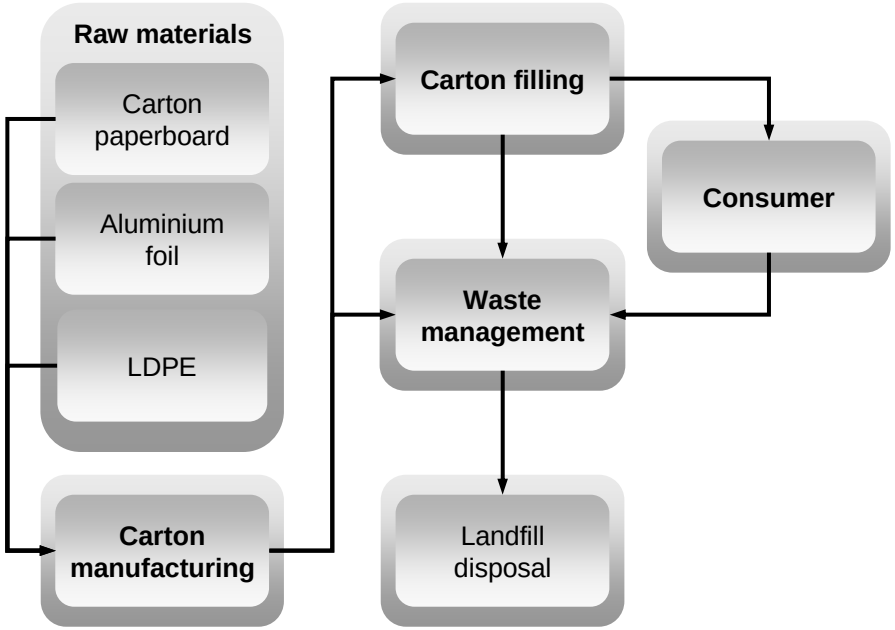
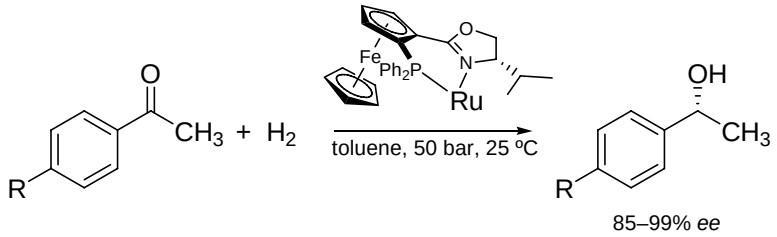
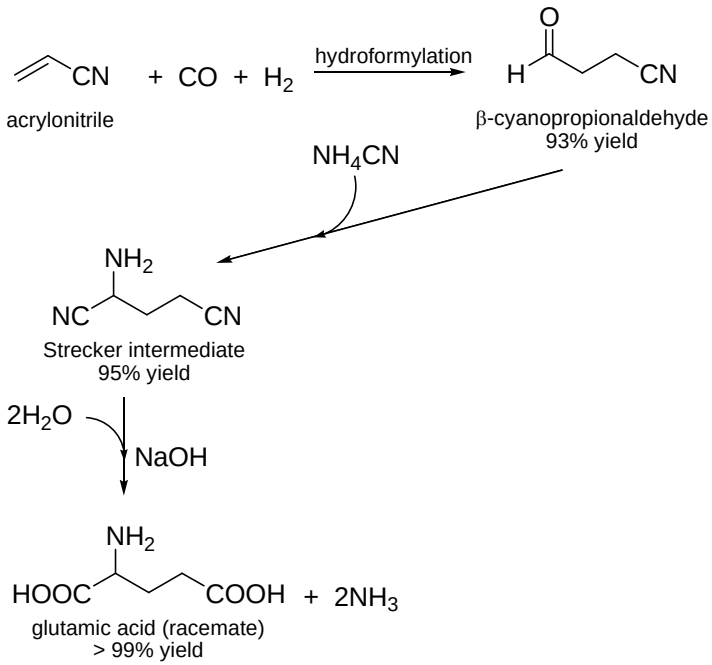

Raw materials
Carton paperboard
Aluminium foil
LDPE
Carton manufacturing
Carton filling
Consumer
Waste management
Landfill disposal

Figure 1.26



R–	substrate:catalyst	time, h	conversion, %
Cl–	50,000	78	99
CH_3O–	20,000	1	92
F–	500	1	100

Figure 1.27


CN
+ CO + H_2
hydroformylation
O
H
CN
acrylonitrile
β-cyanopropionaldehyde
93% yield
NH_4CN
NH_2
NC
CN
Strecker intermediate
95% yield
$2H_2O$
NaOH
NH_2
HOOC
COOH
+ $2NH_3$
glutamic acid (racemate)
> 99% yield