Introduction to Green Chemistry

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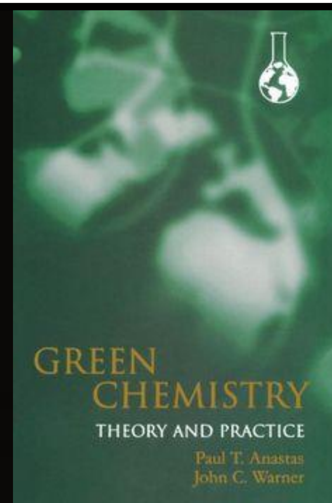
From chemistry …

„If a chemist would manage – in an easy manner – to transform naphtaline into chinine, we would rightly honour him as a benefactor of humanity. Such a transition has not yet been achieved, but from this does not follow that it is impossible."

Sources: J. S. Muspratt, A. W Hofmann, ,,Uber das Toluidin, eine neue organische Basis", Ann. Chem. Pharm. 1845, 54, 1-29; hier S. 3; wikipwdia „August Wilhelm von Hofmann"

… to green chemistry



Paul Anastas, Yale University, Professor of Epidemiology Director of the Center for Green Chemistry and Green Engineering

1998
first published by Oxford U.P.

John Warner, Senior Vice President at Zymergen, Global Sustainability Chair at University of Bath, UK, Co-founder of the non-profit organization Beyond Benign

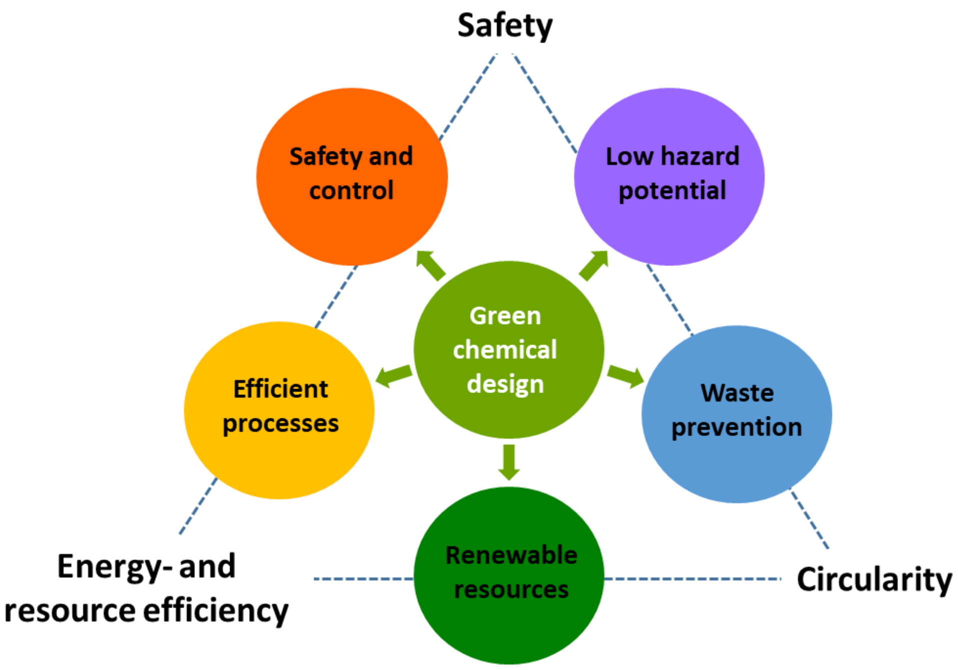
… will receive the Hofmann commemorative medal on September 1 at the EuChemS Chemistry Congress in Lisbon, Portugal.

12 Principles of Green Chemistry

The 12 Principles of Green Chemistry
(Anastas & Warner)

1. Prevent waste
2. Atom Economy
3. Less Hazardous Synthesis
4. Design Benign Chemicals
5. Benign Solvents & Auxiliaries
6. Design for Energy Efficiency
7. Use of Renewable Feedstocks
8. Reduce Derivatives
9. Catalysis (vs. Stoichiometric)
10. Design for Degradation
11. Real-Time Analysis for Pollution Prevention
12. Inherently Benign Chemistry for Accident Prevention

Simplified perspective



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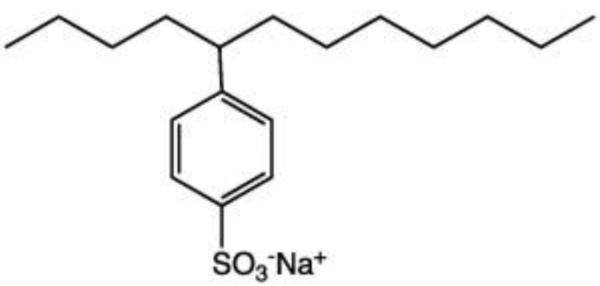
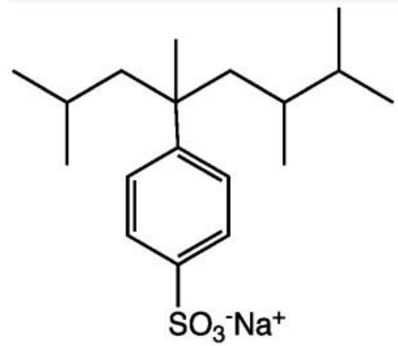
Low hazard potential



vs.



Linear alkyl benzene sulfonates (biodegradable)

Branched alkyl benzene sulfonates (non-biodegradable)

$$2\,\mathrm{MeOH} + \frac{1}{2}\,\mathrm{O_2} + \mathrm{CO} \xrightarrow{\text{Cu salt}} \mathrm{MeOCO_2Me} + \mathrm{H_2O}.$$

vs.

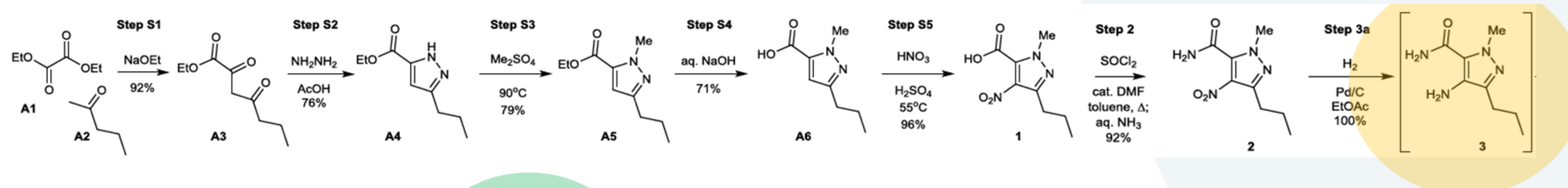
$$COCl_2 + CH_3OH \rightarrow CH_3OCOCl + HCl$$

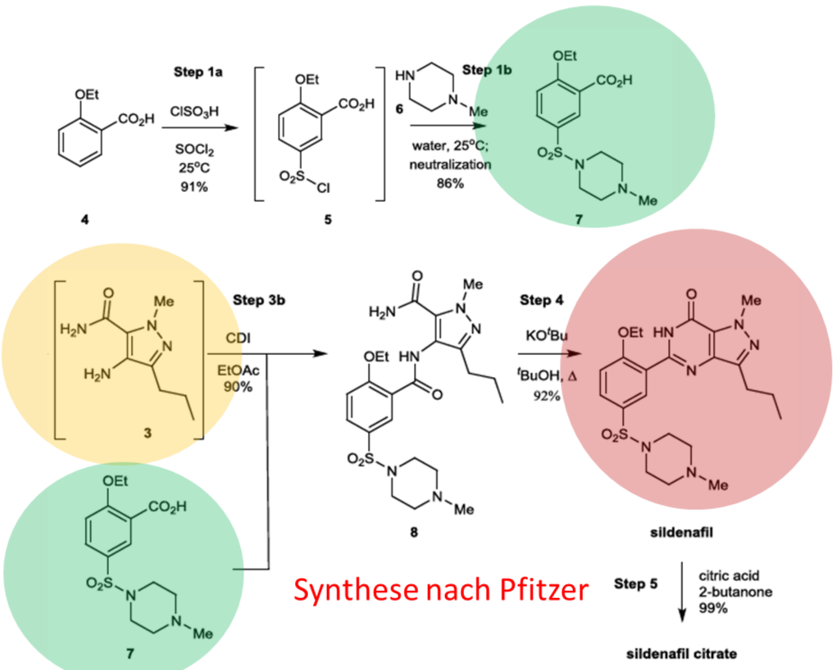
$$CH_3OCOCl + CH_3OH \rightarrow CH_3OCO_2CH_3 + HCl$$

Phosgene-free route to methyl carbonate

Classical phosgene-based route to methyl carbonate

Waste prevention: E = m(waste) / m(product)
The chemical rucksack of a pharmaceutical (Viagra)





Synthese nach Pfitzer

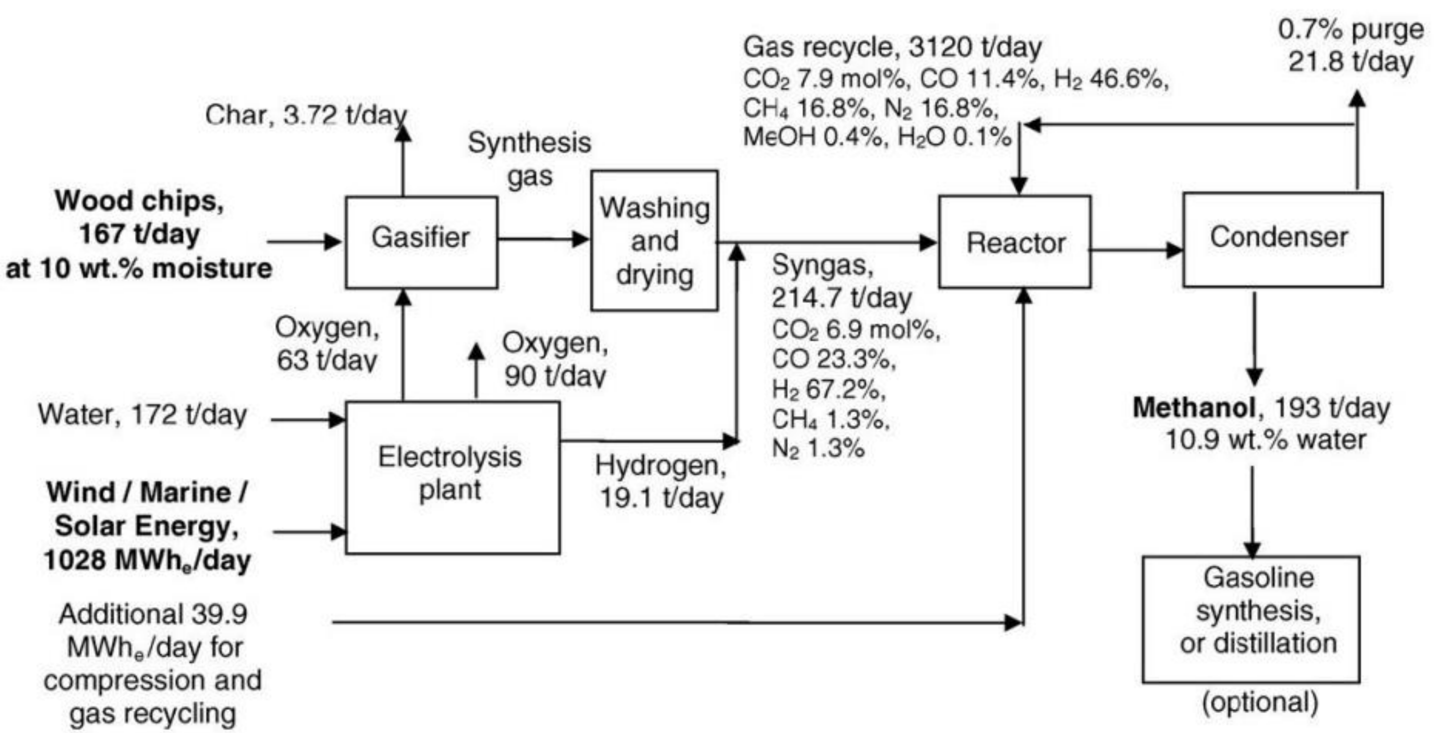
For 1 kg of the product (Viagra) the following amount of ingredients is required:

Raw materials	5,3 kg
Reagents	5,6 kg
Solvents	38,8 kg
Water	85,5

E-factor without water	9,9 kg
E-factor with water	85,5 kg

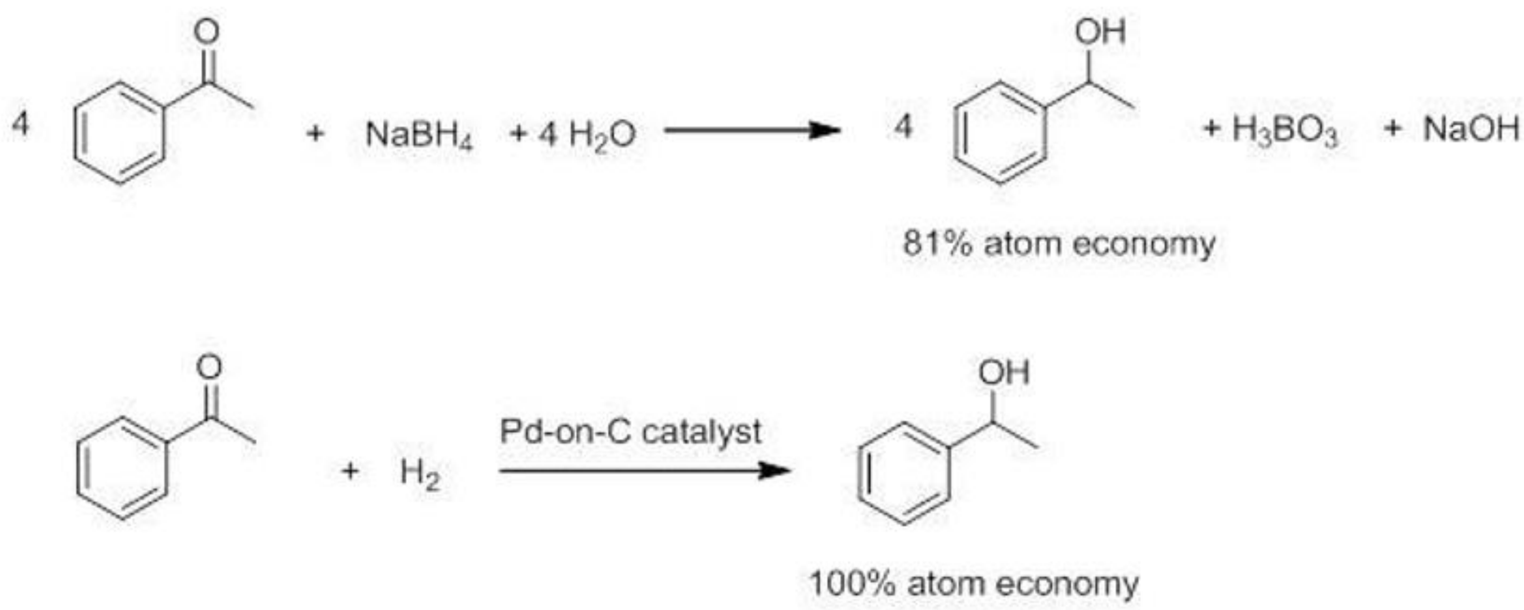
Source: R. Sheldon et al., Green Chemistry, 2014, 1-3

Renewable resources – Methanol synthesis via syngas from biomass



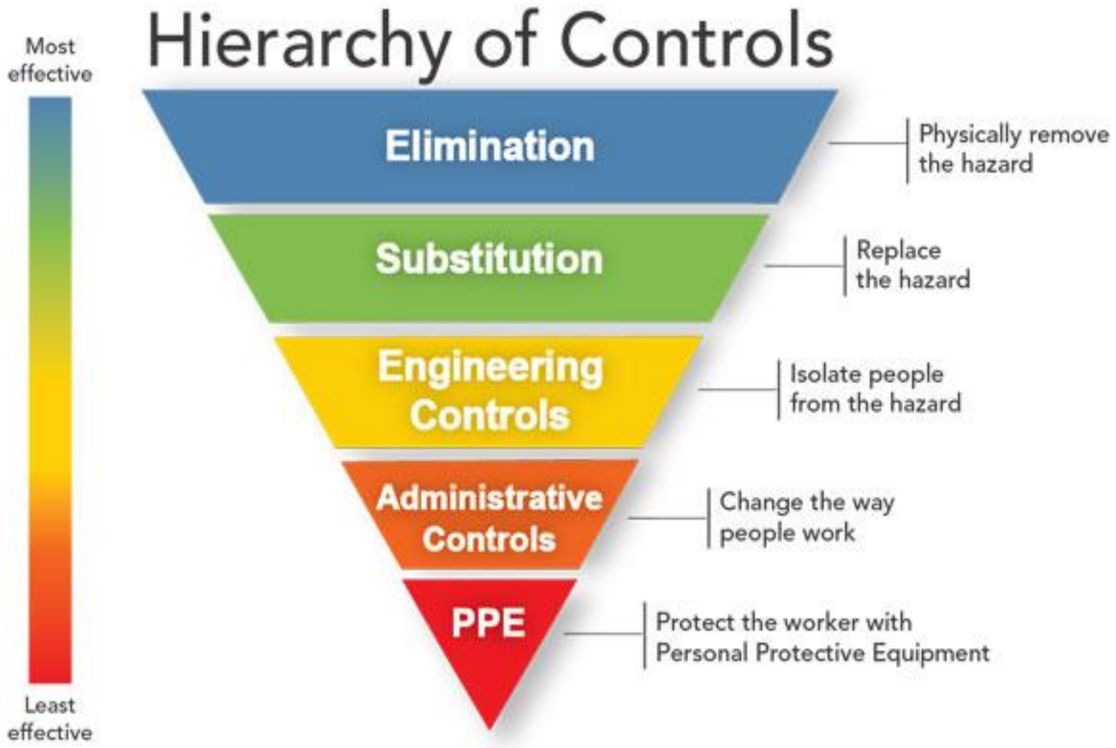
Source: Model by D. Mignard and C Pritchard, publ. in " Chemical Engineering Research and Design (86): 473-487 (2008) . in: Husni Firmansyah, Power and Methanol Production from Biomass Combined With Solar and Wind Energy: Analysis and Comparison, Dissertation, KTH 2018

Efficient processes – Use of catalysts



Source: https://www.acs.org/content/acs/en/greenchemistry/principles/12-principles-of-green-chemistry.html

Safety and control



Substitution potential of Green Chemistry

Definition of green chemistry – an attempt (1)

Green Chemistry is an ecologically oriented chemistry, which follows a holistic approach that integrates the concept of sustainability into every aspect of chemical thinking – from the design and manufacturing of new substances and the processing and use of chemicals down to waste prevention and recycling.

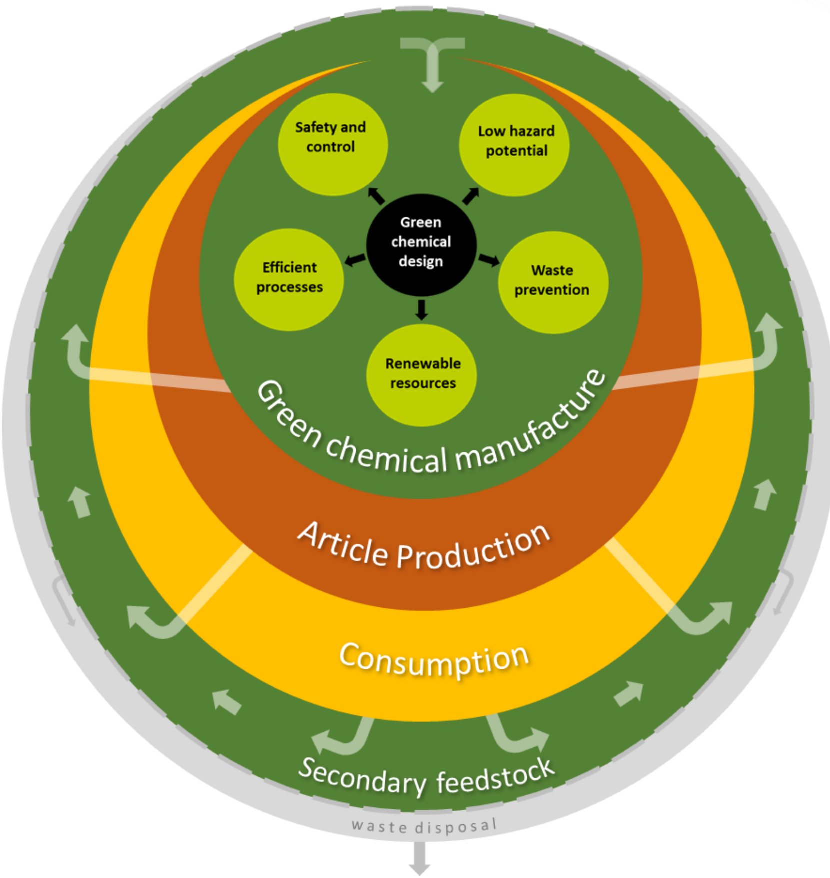
This is the first part of a definition developed by the Austrian platform on Green Chemistry – for more details see https://www.grünechemieösterreich.at/

Definition of green chemistry – an attempt (2)

Green Chemistry is not a new discipline in chemicals science, but an approach which is committed to producing chemicals and using them in a circular manner to the greatest extent possible, based on the principles of protecting human health and the environment and in an energy- and resource-efficient way. It applies this focus from the values imparted to children and their education to research, business and industry practice. The 12 principles of Green Chemistry drafted by John Warner and Paul Anastas are a very useful, concrete, and ambitious roadmap for achieving this future state.

This is the last part of a definition developed by the Austrian platform on Green Chemistry – for more details see https://www.grünechemieösterreich.at/

Green Chemical Design

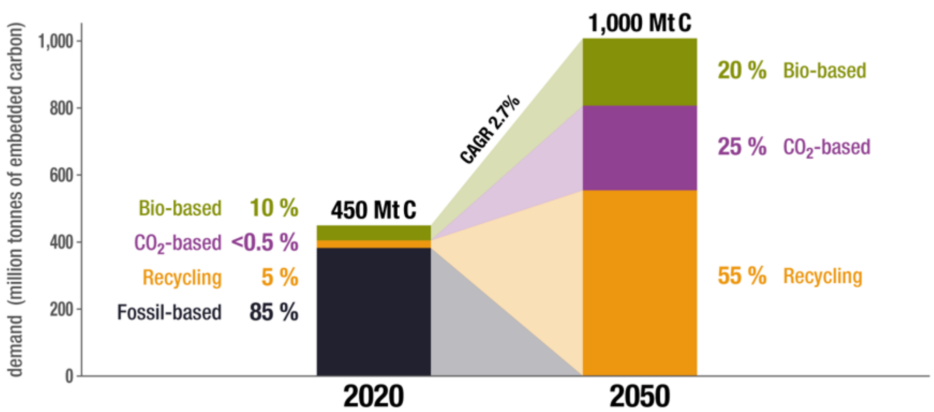


A visualization of the potential key role of Green Chemistry within the production and consumption world.

https://www.grünechemieösterreich.at/

Challenge of defossilisation of the chemical sector

Global Carbon Demand for Chemicals and Derived Materials
in 2020 and Scenario for 2050 (in million tonnes of embedded carbon)



Source: NOVA-Institute

The Austrian chemical industry currently uses mostly fossil raw materials (crude oil, crude gas), amounting to, including mineral and biogenic resources in total ca. 20 Mio. tons, which makes ca. 12 % of the total resource consumption in Austria

(Source: A u. B. Windsperger, Die chemische Industrie auf dem Weg zur Klimaneutralität 2040, St. Pöltern, 2020)

Challenge of defossilisation: alternative carbon sources

- Waste – mechanical or chemical recycling
- Biomass – biorefinery, e.g. pyrolyses to gaseous raw materials such as syngas, or fermentation to alcohols or other organic base materials
- CO_2 – capture and utilization (CCU) using green hydrogen
- CO_2 – capture and storage (directly underground or indirectly via biochar)

The current challenge for the Austrian climate policy is to establish and design a practical roadmap for the transition of the chemical sector to these raw materials. Green chemistry should provide the technical basis for achieving the very ambitious goal of defosilisation in the first half of this century.

Bundesministerium
Klimaschutz, Umwelt,
Energie, Mobilität,
Innovation und Technologie

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Thank you for your attention!

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