NOP - An international organic chemistry lab course for sustainability

2nd International Green and Sustainable Chemistry Meeting

Hotel Washington

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Burkhard Koenig

What is NOP?

- A common project of 6 German Universities from 2000 - 2003

What is NOP?

- A common project of 6 German Universities from 2000 - 2003
- Selection of experiments

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- A common project of 6 German Universities from 2000 - 2003
- Selection of experiments
- Adaption, testing and evaluation

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- A common project of 6 German Universities from 2000 - 2003
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- Background information

What is NOP?

- A common project of 6 German Universities from 2000 - 2003
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- Website development

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... and then go international!

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Prof. B. Jastorff, Frau A. Müller,
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Prof. P. Tundo

NOP

- **N** stands for Nachhaltigkeit (sustainability)

NOP

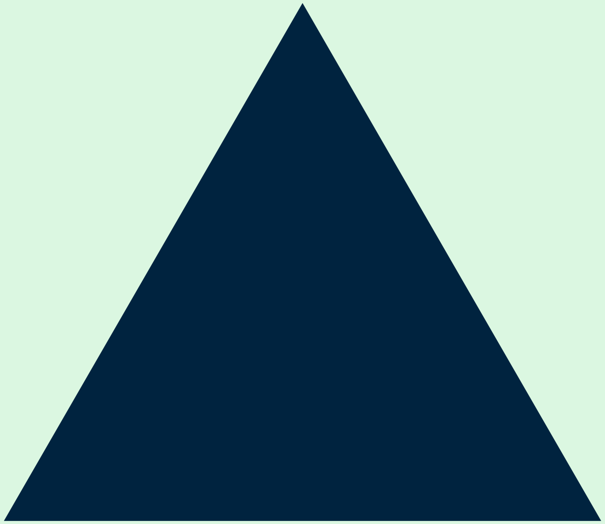
- **N** stands for Nachhaltigkeit (sustainability)
- **O** stands for Organic chemistry

NOP

- **N** stands for Nachhaltigkeit (sustainability)
- **O** stands for Organic chemistry
- **P** stands for Praktikum (lab course)

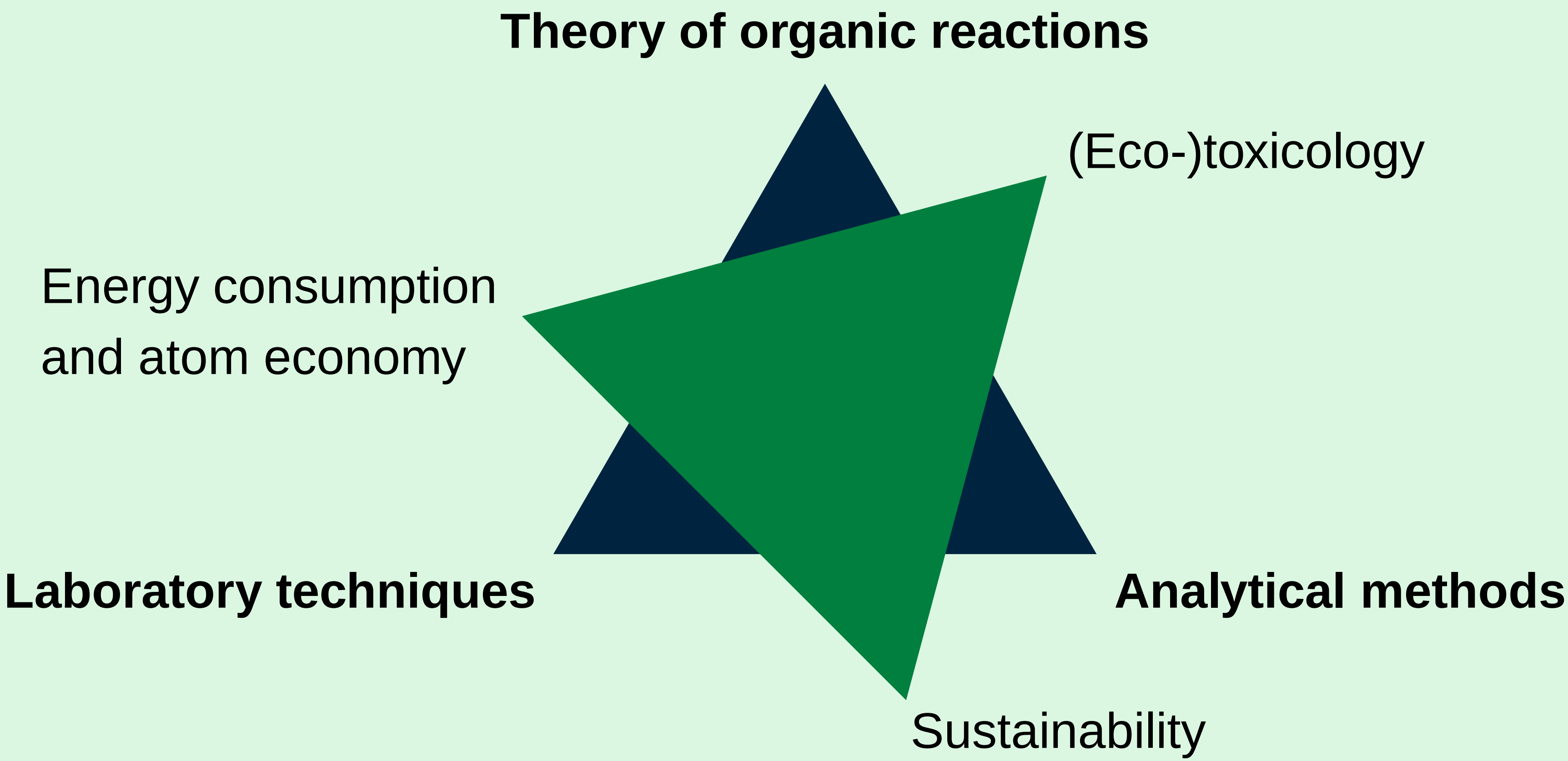
Concept

Theory of organic reactions



Laboratory techniques **Analytical methods**

Concept


Theory of organic reactions
(Eco-)toxicology
Energy consumption and atom economy
Laboratory techniques
Analytical methods
Sustainability

Elements of the NOP

- Experimental instructions

Elements of the NOP

- Experimental instructions
- Information on evaluation of substances and reactions

Elements of the NOP

- Experimental instructions
- Information on evaluation of substances and reactions
- Background articles

Criteria for experiment selection

- Coverage of laboratory techniques

Criteria for experiment selection

- Coverage of laboratory techniques
- Coverage of reaction types

Criteria for experiment selection

- Coverage of laboratory techniques
- Coverage of reaction types
- Alternative methods

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- Alternative methods
- High stoichiometric yield

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- High stoichiometric yield
- High chemo-, regio-, and stereoselectivity

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- High chemo-, regio-, and stereoselectivity
- High energy efficiency

Criteria for experiment selection

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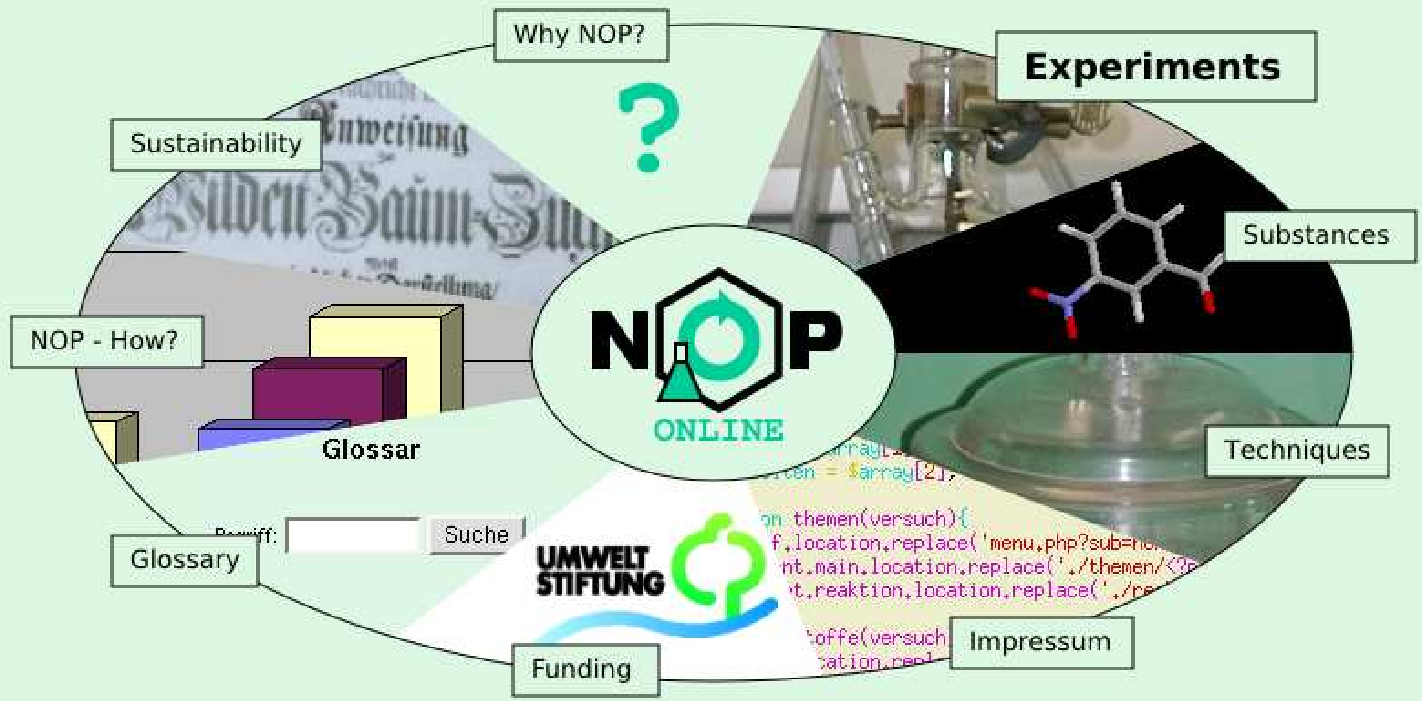
- High stoichiometric yield
- High chemo-, regio-, and stereoselectivity
- High energy efficiency
- High substance efficiency

Criteria for experiment selection

- Coverage of laboratory techniques
- Coverage of reaction types
- Alternative methods
- High stoichiometric yield
- High chemo-, regio-, and stereoselectivity
- High energy efficiency
- High substance efficiency
- Low substance risk potential

Welcome!

Sustainability in the organic chemistry lab course



For optimal viewing of the NOP pages JavaScript has to be activated in your browser and the Chime plugin must be installed. The pages were optimized for a screen resolution of 1024 x 768. Help with the installation of Chime with newer browsers is available.

English | Change language

pages/entry.php: June 17, 2005
en/inc/entry.html: February 11, 2005

Why a new lab course?

The NOP wants to convey ...

... modern organic chemistry including alternative methods

Why a new lab course?

The NOP wants to convey ...

... modern organic chemistry including alternative methods

... a feeling for substance risks

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The NOP wants to convey ...

... modern organic chemistry including alternative methods

... a feeling for substance risks

... a feeling for the environmental load

Why a new lab course?

The NOP wants to convey ...

... modern organic chemistry including alternative methods

... a feeling for substance risks

... a feeling for the environmental load

... the concept of sustainable development

Sustainability


Background information on sustainable development

[HTML] Summary

[HTML] What is the meaning of sustainability?

[HTML] History of sustainability

[HTML] Economic rules

[HTML] Ecological rules

[HTML] Social rules

[HTML] Sustainability in chemistry

[HTML] Further readings

W3C XHTML 1.0 W3C css SOME RIGHTS RESERVED English Change language *pages/sustainability.php*: *March 15, 2005*

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Version control

[nop] / www / pages / sustainability.php   Project Root: nop Go

View of /www/pages/sustainability.php

ViewCVS

Parent Directory | Revision Log

Revision: **181** - (**download**) (**as text**)
Tue Mar 15 14:09:56 2005 UTC (3 months ago) by *ranke*
File size: 723 byte(s)

```
Checked the validity of our XHTML, and made a lot of small corrections, especially
to the experiment evaluation texts.
```

```php
<?php
include 'inc/logohead.inc';
include 'functions/articlegroup.php';

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<table class='centered' width='50%'>
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    translate("Background information on sustainable development"); echo
"</h3></td></tr>
<tr><td>";
    articlegroup(array(
        "sustainability;summary;Summary",
```

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Sustainability

Summary

What is the meaning of sustainable development?

The history of sustainable development

Economic rules

Ecological rules

Social rules

Sustainability in chemistry

References

Sustainability in chemistry

Chemistry in the context of sustainable development is at the same time a chance and a risk. The risks are high, as demonstrated by the accidents at Seveso in Italy, Bophal in India and at Sandoz Corp. in Basle, Switzerland. Also, seemingly less important effects like the ubiquitous emission and accumulation of POPs (persistent organic pollutants), have their origin in the chemical industry.

Besides these dangers, chemistry offers great potentials for sustainable development [12]. The chemical industry can support the development towards a more sustainable lifestyle of society according to its competence in the field of transformation of products and materials.

The production of insulation material for public and private buildings is a good example of the contributions chemistry has made in this process. The energy necessary for the production of these materials is conserved within the first year of operation by reduced heating needs [13]. A long-term reduction of the energy used for heating buildings has become possible. Another example is the development of catalytic converters for motor vehicles, which led to a great reduction in emissions. This in turn has lead to a significant improvement of environmental air quality. In the following chapters, the stands and statements of trade unions and of chemical industry regarding the issue of sustainable development will be discussed.

Perspective of the environmental organzations

Today, there are detailed regulations imposed by the legislation of most modern states regarding environmental issues like the handling of chemical compounds and maintenance of chemical plants. These regulations are the result of the controversial discussions in the 1980s about the role of chemistry. The former social explosiveness expressed, e.g. by reports like "Seveso ist überall" (Seveso is everywhere) [14] has cooled down. In addition, environmental NGOs have

Sustainability international

NOP ONLINE

Sommario

Che cosa significa sviluppo sostenibile?

Storia dello sviluppo sostenibile

Economic rules

Regole ecologiche

Regole sociali

La sostenibilità nella chimica

Riferimenti bibliografici

La sostenibilità nella chimica

La chimica in un contesto di sviluppo sostenibile rappresenta, al tempo stesso, un'opportunità ed un pericolo. I rischi sono seri come dimostrato dagli incidenti di Seveso in Italia, Bophal in India e alla società Sandoz di Basilea in Svizzera. Vanno inoltre considerate le emissioni di inquinanti organici persistenti (solitamente indicati con l'abbreviazione POP o POPs, dall'inglese Persistent Organic Pollutants; n.d.t.) da parte delle industrie chimiche. Tali emissioni sono ubiquitarie e i contaminanti rilasciati spesso tendono ad accumularsi nell'ambiente.

Eppure, oltre a presentare tali pericoli, la chimica offre grandi applicazioni potenziali per lo sviluppo sostenibile [12]. L'industria chimica può favorire l'adozione di uno stile di vita più sostenibile, mettendo a disposizione le sue competenze nel campo della trasformazione dei materiali e dei prodotti.

Un buon esempio di quanto appena esposto sono i materiali isolanti usati negli edifici pubblici e privati. L'energia richiesta per la loro produzione viene recuperata in un solo anno grazie alla minor richiesta di energia degli impianti di riscaldamento [13]. Diviene così possibile una riduzione a lungo termine dell'energia usata per il riscaldamento degli edifici. Un altro esempio è quello dell'introduzione delle marmitte catalitiche per gli autoveicoli che ha portato ad una notevole diminuzione nell'emissione di inquinanti, che si riflette in un miglioramento della qualità dell'aria.

Nei prossimi paragrafi descriveremo le posizioni e le dichiarazioni di vari soggetti e dell'industria chimica in relazione allo sviluppo sostenibile.

Il punto di vista delle organizzazioni ambientali

Attualmente la maggior parte degli stati moderni ha emesso normative dettagliate in materia di protezione ambientale, che riguardano, ad esempio, la manipolazione dei composti chimici e la manutenzione degli impianti chimici. Tali leggi sono il risultato di discussioni controverse circa il ruolo della chimica che risalgono agli anni '80.

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Sustainability international

- Zusammenfassung
- Was ist Nachhaltigkeit
- Geschichte der Nachhaltigkeit
- Ökonomische Regeln
- Ökologische Regeln
- Gesellschaftliche Regeln
- Nachhaltigkeit in der Chemie
- Literatur

Nachhaltigkeit in der Chemie

Die Chemie ist für das Konzept der nachhaltigen Entwicklung Chance und Gefahr zugleich. Die mit Chemie im Zusammenhang stehenden Gefahren sind groß und zeigen sich bei Unfällen wie in Seveso, Bophal oder bei Sandoz. Auch auf den ersten Blick weniger dramatische Auswirkungen, wie z.B. die ubiquitäre Verbreitung von POPs (Persistent organic pollutants) haben ihren Ursprung zum Teil in der chemischen Industrie. Neben diesen Gefahren, bietet die Chemie aber auch große Potenziale für eine nachhaltigere Entwicklung [12]. Durch die Kompetenz dieses Industriezweiges auf dem Gebiet der Stoffumwandlung können wichtige Teilbereiche bei der Entwicklung hin zu einer nachhaltigen Gesellschaft mitgestaltet werden. Ein herausragendes Beispiel hierzu ist die Herstellung von Isoliermaterialien zur Gebäudedämmung. Die zur Herstellung der Dämmmaterialien verbrauchte Energie kann oft schon nach einem Jahr durch verringerte Energieverluste eingespart werden [13], eine langfristige Reduktion des Energieverbrauchs aus der Gebäudeheizung wurde dadurch erst möglich gemacht. Auch die Entwicklung von Katalysatoren, z.B. für den Kraftfahrzeugbereich brachte große Reduktionen der Emissionslasten und damit eine Verbesserung der Umweltsituation. Wie Umweltverbände und Chemieindustrie auf die Forderungen nach einer "Nachhaltigen Entwicklung" reagieren, soll in den folgenden Abschnitten geklärt werden.

Sichtweise der Umweltverbände

Im Zuge der stark kontroversen Diskussionen um Chemie, die in den 80er Jahren geführt wurden, ist auch ein umfangreiches staatliches Regelwerk zum Umgang mit chemischen Stoffen und chemischen Produktionsanlagen entstanden. Die gesellschaftliche Brisanz, die sich z.B. in Berichten wie "Seveso ist überall" [14] niederschlug, ist bei weitem nicht mehr so groß. Überdies werden die Umweltverbände heute in die chemiepolitischen Entscheidungen eingebunden. Weiterhin ist zu beobachten, dass andere Diskussionen, wie z.B. die Diskussionen

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NOP - How?

[HTML] Short introduction to the contents of NOP

Legal requirements

- Gesetzliche Rahmenbedingungen für den Umgang mit Gefahrstoffen
- Technical directives for lab courses
- Operating instructions for lab courses
- Risk and Safety phrases
- Hazard Symbols
- Chemical waste evaluation and classification

Evaluation methods for chemical substances and reactions

- [HTML] Preliminary remarks to the articles about evaluation methods
- [HTML] Indices for synthesis reactions
- [HTML] Evaluation of chemical substances
- Die Methode der Ökobilanzierung
- Input Analysis of chemical reactions
- Ökobilanz - Beispiel 1
- Ökobilanz - Beispiel 2
- [HTML] Integrated evaluation of chemical syntheses

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Laboratory techniques

Laboratory techniques

- Arbeitsmethoden im Laboratorium
- Sustainable synthesis optimization rules
- Alternative methods of energy input: Microwave technology
- Technical instructions for hot extraction filtration in microwave ovens
- Technical instructions for the standard reflux apparatus in microwave ovens
- Used solvents in the laboratory: Disposal and/or recycling?
- Treatment and disposal of laboratory waste
- Chromatographische Analysenmethoden
- Spektroskopische Methoden
- Environmental aspects of using vacuum
- Environmental aspects of introducing energy into reaction mixtures

English Change language

pages/techniques.php: October 29, 2004

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Glossary

Glossary

Search term: energy Search Show all

A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

Term	Definition	Article	Compare
energy efficiency:	Mass of the purified product per kJ of invested energy. The energy efficiency of a synthesis is strongly dependent on the equipment used, the experimentalist, and the preparation size.		mass efficiency
energy-induced methane equivalents:	This key value describes the ratio of the amount of methane that must be burnt in a model energy plant to generate enough energy to perform a specific reaction to the mass of the generated product.		

English Change language

pages/glossary.php: *December 23, 2004*

Experiments

Experiments

Search category | Search term | Degree of difficulty

Substance classes | acetal | Easy | Search

Every occurrence of the search term in the chosen category will lead to a hit

Experiments that are part of the NOP teaching module are shown on a grey background

Show all experiments | All degrees of difficulty

NOP-No	Title	Substance classes	Reaction type	Work methods	Difficulty
2003	**Acid catalyzed acetalisation of 3-nitrobenzaldehyde with ethanediol to the correspondent 1,3-dioxolane**	aldehyde, acetal, alcohol, protecting group, acid catalyst	reaction of the carbonyl group in aldehydes, acetalisation	removal of water by azeotropic distillation, heating under reflux with Soxhlet extractor (for 10 mmol preparation), stirring with magnetic stir bar, evaporating with rotary evaporator, shaking out, extracting, recrystallizing, filtering, heating with oil bath	Easy
2002	**Acid catalyzed acetalisation of acetoacetic acid ethyl ester with ethanediol to the corresponding 1,3-dioxolane**	ketone, alcohol, acetal, protecting group, acid catalyst	reaction of the carbonyl group in ketones, acetalisation	removal of water by azeotropic distillation, stirring with KPG stirrer, filtering, evaporating with rotary evaporator, distilling under reduced pressure, fractionating column distillation, rectifying, heating with oil bath, stirring with magnetic stir bar	Easy
2005	**Synthesis of the acetonide of meso-1,2-diphenyl-1,2-ethanediol (2,2-dimethyl-4,5-diphenyl-1,3-dioxolane)**	ketone, alcohol, acetal, protecting group, acid catalyst	reaction of the carbonyl group in ketones, acetalisation	heating under reflux, stirring with magnetic stir bar, filtering, evaporating with rotary evaporator, shaking out, extracting, recrystallizing, working with moisture exclusion, heating with oil bath	Easy

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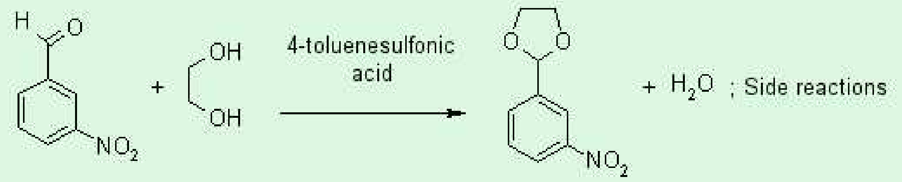
Example



NOP-Nr: 2003

Alternative: 5004

Overview
Instructions
Operating scheme
Substances
Equipment
Evaluation
Analytics
User comments

Acid catalyzed acetalisation of 3-nitrobenzaldehyde with ethanediol to the correspondent 1,3-dioxolane

Reaction type:	reaction of the carbonyl group in aldehydes, acetalisation
Substance classes:	aldehyde, acetal, alcohol, protecting group, acid catalyst
Work methods:	removal of water by azeotropic distillation, heating under reflux with Soxhlet extractor (for 10 mmol preparation), stirring with magnetic stir bar, evaporating with rotary evaporator, shaking out, extracting, recrystallizing, filtering, heating with oil bath
Degree of difficulty:	Easy

English Change language

pages/experiment.php: February 14, 2005
views/overview.php: December 21, 2004

Instructions

NOP-Nr: 2003
Alternative: 5004

- Overview
- Instructions
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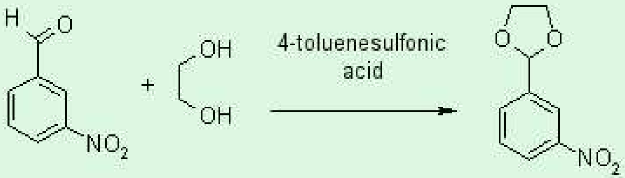
- User comments



Synthesis instructions as PDF file for printing

Acid catalyzed acetalisation of 3-nitrobenzaldehyde with ethanediol to the correspondent 1,3-dioxolane

Batch scale: 0.1 mol 0.01 mol 3-Nitrobenzaldehyde

Reaction

3-Nitrobenzaldehyde (15.1 g, 100 mmol), ethanediole (6.83 g, 6.20 mL, 110 mmol) and 4-toluenesulfonic acid monohydrate (1.00 g, 5.30 mmol) are dissolved in cyclohexane (200 mL) in a dry 500 mL round bottom flask equipped with magnetic stirring bar, Dean Stark trap and reflux condenser. The reaction mixture is refluxed until no more water is collected in the Dean-Stark trap (approx. 2-3 h).

Work up

The hot reaction mixture is poured into another 500 mL round bottom flask to separate it from an oily sediment (800 mg) which has formed at the bottom of the reaction vessel. The sediment consists predominantly of product, starting material and 4-toluenesulfonic acid (^{1}H-NMR spectrum). The solvent of the decanted solution is directly removed with a rotary evaporator . A yellow crystalline solid remains as crude product.

Crude product yield: 19.7 g; melting point 50-52 °C; Purity according to GC: 95% acetale + 4% aldehyde

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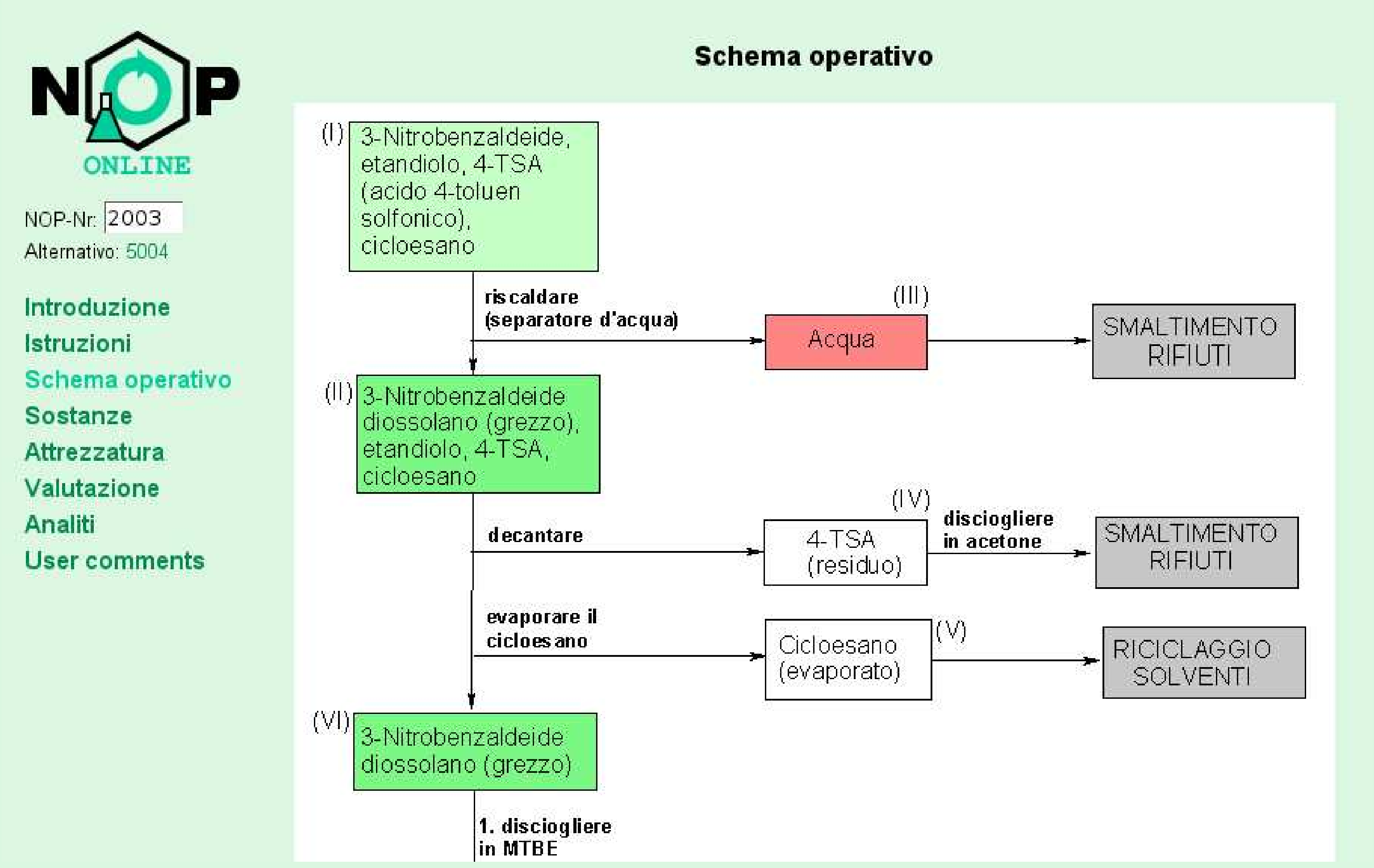
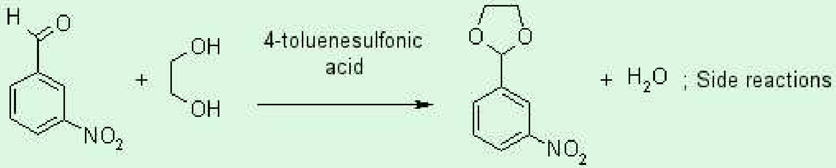
Operating scheme



Required substances

NOP-Nr: 2003
Alternative: 5004

- Overview
- Instructions
- Operating scheme
- Substances
  - Substances required
  - Substances produced
  - Data availability
  - Effect factors TRGS 440
  - Stoichiometry
- Equipment
- Evaluation
- Analytics
- User comments



Substances required

Batch scale: (•) 0.1 mol ( ) 0.01 mol 3-Nitrobenzaldehyde

Educts		**Amount**	**Risk**	**Safety**
3-Nitrobenzaldehyde	Xn	15.1 g	R 22-36/37/38	S 22-24/25-26-36
1,2-Ethanediol	Xn	6.83 g	R 22	S 2
Catalyst		**Amount**	**Risk**	**Safety**
4-Toluenesulfonic acid monohydrate	Xi	0.19 g	R 36/37/38	S 2-26-37
Solvents		**Amount**	**Risk**	**Safety**
Cyclohexane	F Xn N	~ 230 mL	R 11-38-50/53-65-67	S 2-9-16-33-60-61-62
tert-Butyl methyl ether	F Xi	230 mL	R 11-38	S 2-9-16-24
Others		**Amount**	**Risk**	**Safety**
Sodium disulfite	Xn	~ 13 g	R 22-31-41	S 2-26-39-46
Sodium sulfate	Xi	~ 5 g	R 36/37/38	S 26-36
Molecular sieve 4A	Xi	0 g	R 36/37/38	S 24/25

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Substances produced

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NOP-Nr: 2003
Alternative: 5004

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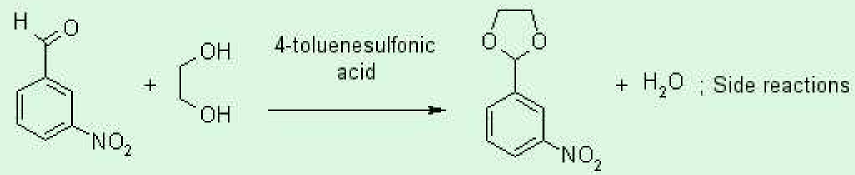

Substances produced

Batch scale: (•) 0.1 mol ( ) 0.01 mol 3-Nitrobenzaldehyde

Products	Amount	Risk	Safety
2-(3-Nitrophenyl)-1,3-dioxolane	17.9 g	R no data	S no data
Water		R	S

Waste	Disposal
aqueous phase from water separator	solvent water mixtures, halogen free
aqueous phase from shaking out	solvent water mixtures, halogen free
dissolve residue from reaction flask in a small amont of acetone	organic solvents, halogen free
mother liquor from recrystallisation	organic solvents, halogen free
sodium sulfate	solid waste, free from mercury

English | Change language

pages/experiment.php: *February 14, 2005*
views/produced.php: *March 01, 2005*

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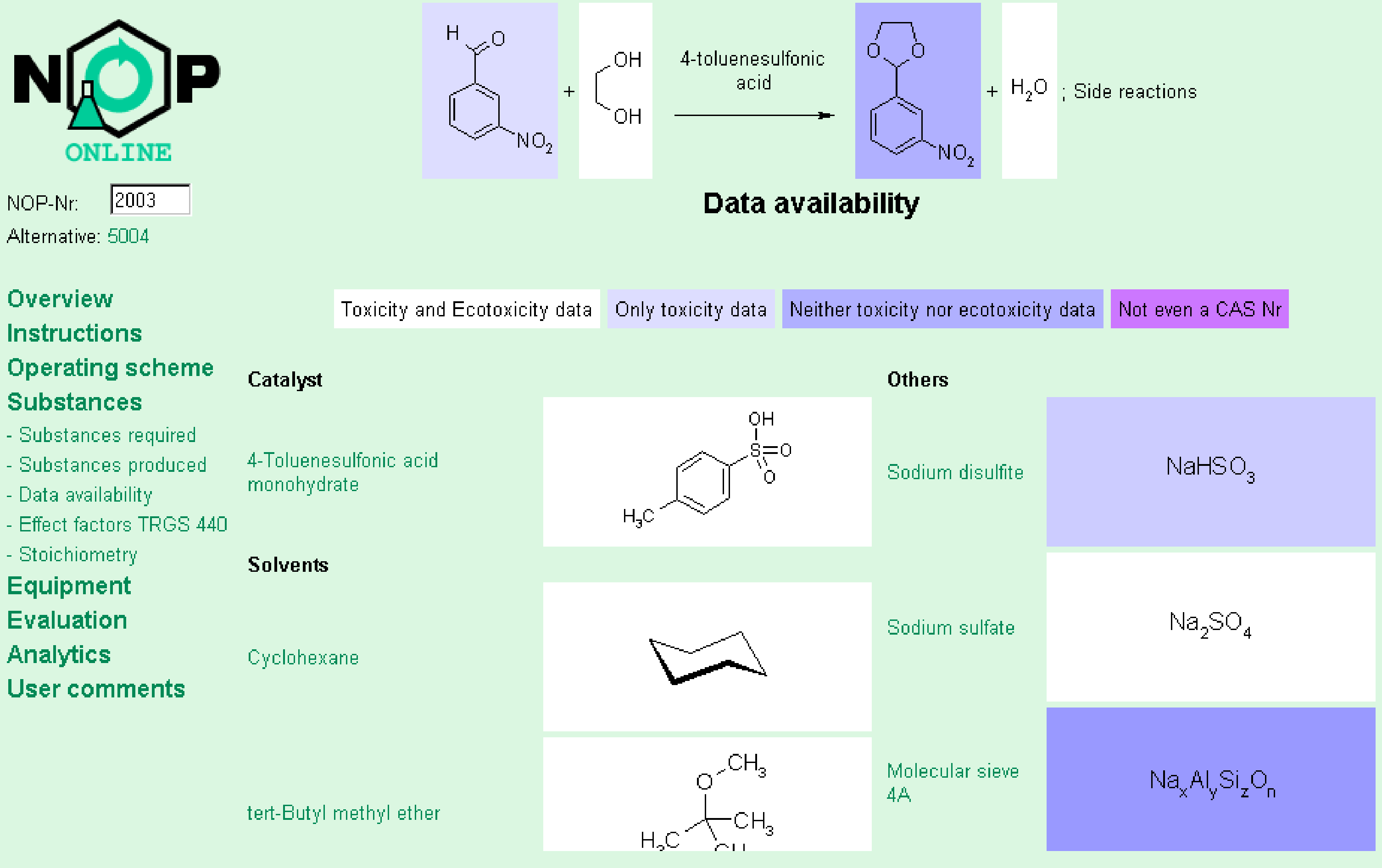
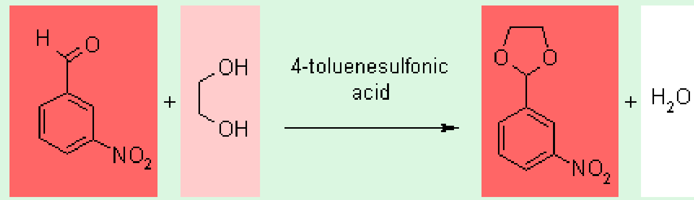
Data availability



Effect factors

NOP-Nr: 2003

Alternative: 5004

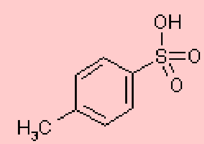


Effect factors TRGS 440

Effect factor 0	Effect factor >0 to 10	Effect factor >10 to 100	Effect factor >100 to 1000	Effect factor >1000 to 50000

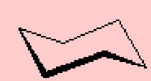
Catalyst

4-Toluenesulfonic acid monohydrate
Effect factor: 5

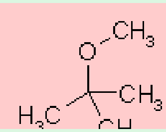


Solvents

Cyclohexane
Effect factor: 5



tert-Butyl methyl ether
Effect factor: 5



Others

Sodium disulfite
Effect factor: 100

$NaHSO_3$

Sodium sulfate
Effect factor: 5

Na_2SO_4

Molecular sieve 4A
Effect factor: 5

$Na_xAl_ySi_zO_n$

Equipment

NOP-Nr: 2003

Alternative: 5004

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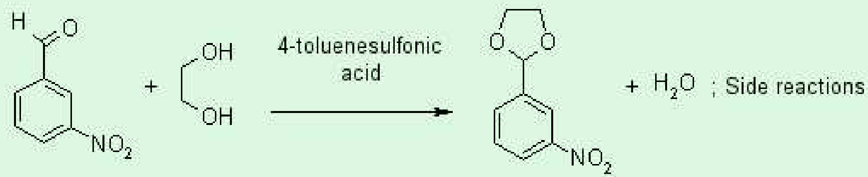

Equipment

Batch scale: (•) 0.1 mol ( ) 0.01 mol 3-Nitrobenzaldehyde


round bottom flask 500 mL


water separator


reflux condenser


heatable magnetic stirrer with magnetic stir bar


separating funnel


rotary evaporator

Evaluation indices

NOP-Nr: 2003

Alternative: 5004

- Overview
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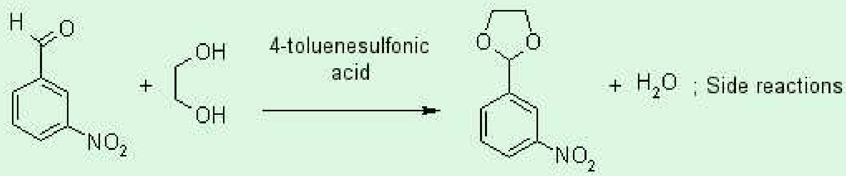

Simple evaluation indices

Batch scale: 0.1 mol 0.01 mol 3-Nitrobenzaldehyde

Atom economy	91.5 %
Yield	92 %
Target product mass	17.9 g
Sum of input masses	390 g
Mass efficiency	46 mg/g
Energy input	2500 kJ
Energy efficiency	7.2 mg/kJ

English Change language

pages/experiment.php: February 14, 2005
views/indices.php: February 05, 2005

Evaluation texts

NOP-Nr: 2003

Alternative: 5004

- Overview
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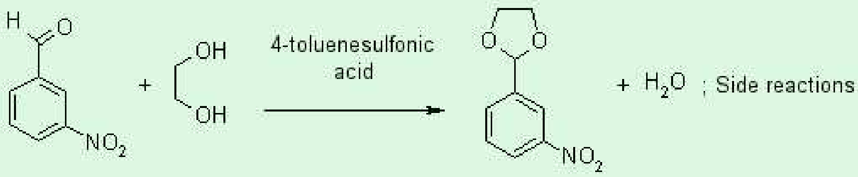
- Substances
- Equipment
- Evaluation
  - Indices
  - Evaluation text
- Analytics
- User comments



Evaluation text

The classical variant of the "Acid catalyzed acetalisation of 3-nitrobenzaldehyde with ethanediol to the correspondent 1,3-dioxolane" is an easily performed experiment. The desired product is obtained in high yield and high selectivity. Also the purity of the end product is very high.

The mass efficiency is high to medium, compared to the other NOP experiments and thus evaluates as good. The energy efficiency of the classical experiment is highly dependent on the method of heating.

(Eco)toxicological data for the educt 3-nitrobenzaldehyde are incomplete, toxicological data for the product 2-(3-nitrophenyl)-1,3-dioxolane have not been determined at all. According to theoretical prediction methods both product and educt are suspected to have mutagenic, carcinogenic and sensitizing properties. The organic solvents used in this experiment ethanol, cyclohexane and tert-butyl methyl ether exhibit relatively low acute toxicity. Also the inorganic auxiliary materials do not pose significant dangers to human health.

Educt, product and the solvents cyclohexane and tert-butyl methyl ether are biologically not easily degradable, and some are classified as dangerous to the environment because of their toxicity to aquatic organisms.

Summed up we evaluate this experiment with a good economic efficiency and acceptable toxicological risks, but a relatively high environmental persistence of the used substances with the "yellow light".

English Change language

pages/experiment.php: *February 14, 2005*
en/exp_evaluations/html/2003.html: *March 15, 2005*

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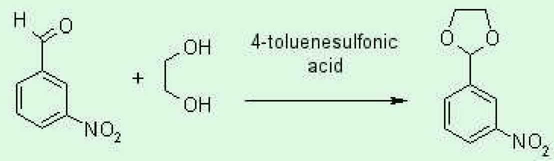
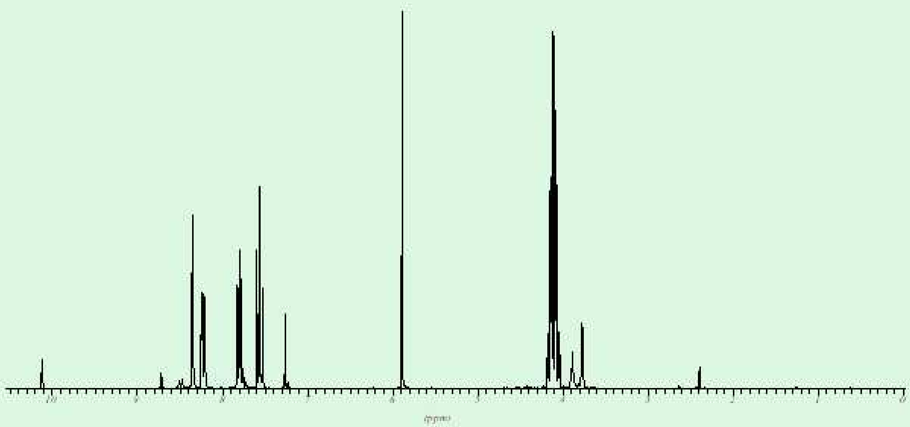
Analytics

NOP-Nr: 2003
Alternative: 5004

- Overview
- Instructions
- Operating scheme
- Substances
- Equipment
- Evaluation
- Analytics
  - Chromatogram
  - ^{1}H-NMR
  - ^{13}C-NMR
  - IR
- User comments

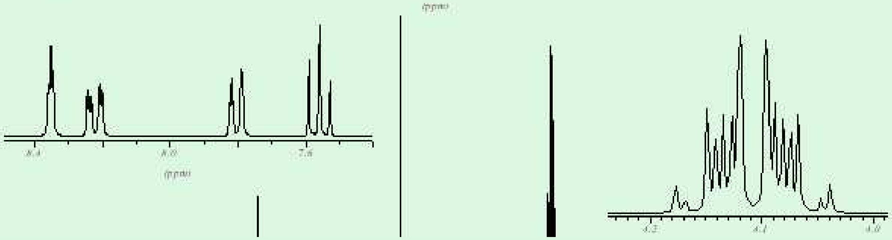


^{1}H-NMR



^{1}H-NMR: crude product
250 MHz, $CDCl_3$

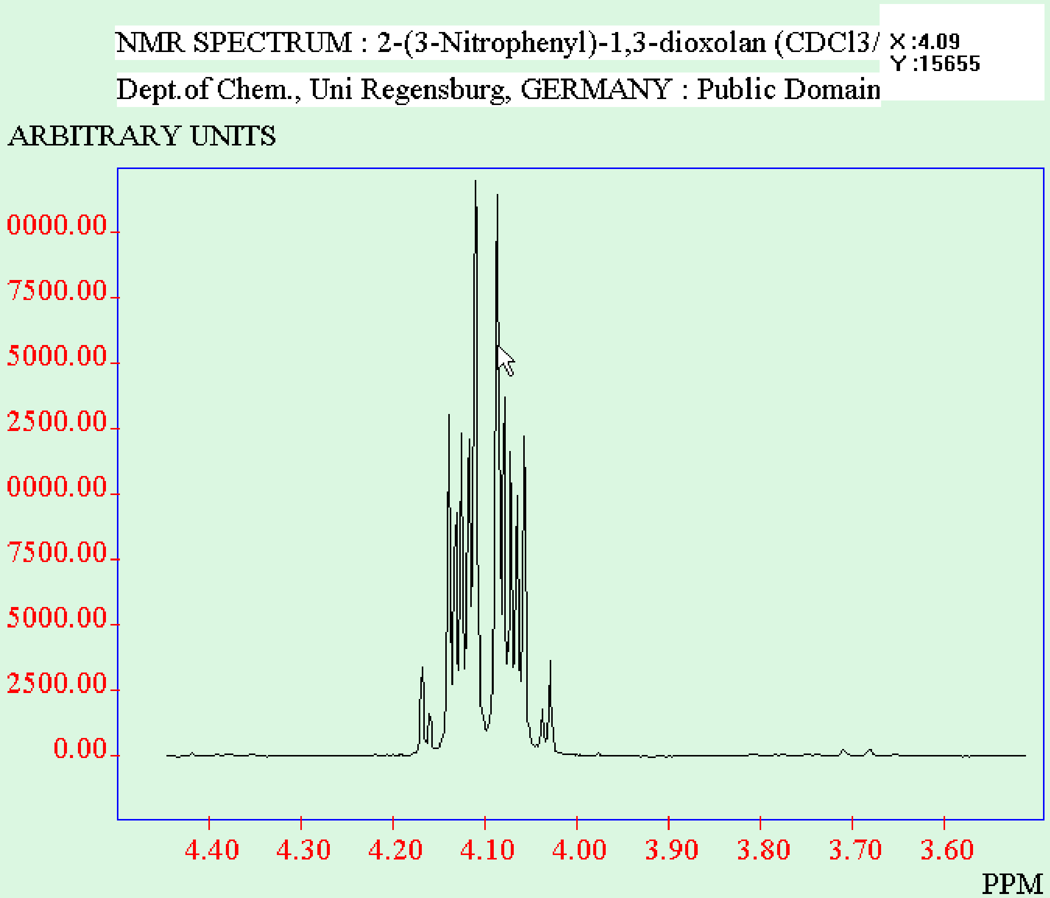
delta [ppm]	mult.	atoms	assignme
4.05-4.18	m	4 H	$-OCH_2CH$
5.90	s	1 H	O-CH-O
7.54-7.60	m	1 H	5-H
7.79-7.83	m	1 H	6-H
8.20-8.25	m	1 H	4-H
8.35-8.37	m	1 H	2-H
7.26			$CHCl_3$
10.15	s	1 H	CHO (edu

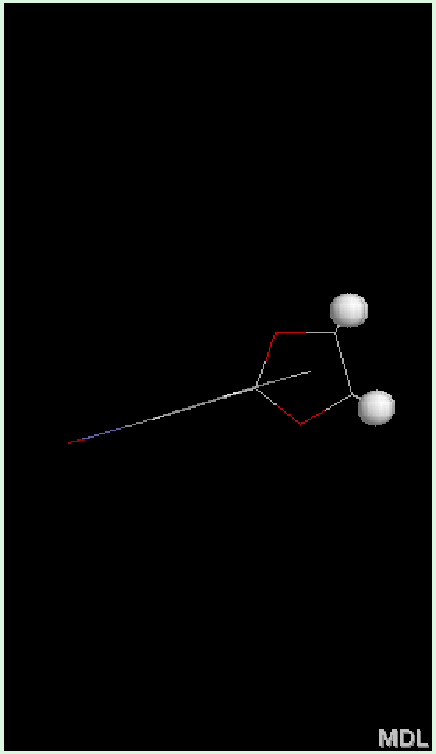


^{1}H-NMR:
2-(3-Nitrophenyl)-1,3-dioxolane
250 MHz, $CDCl_3$
interactive spectrum

delta [ppm]	mult.	atoms	assignme
4.05-4.18	m	4 H	$-OCH_2CH$

Interactive spectra

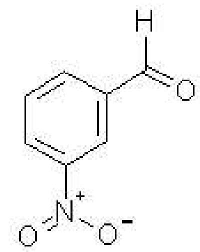




Substances

Example

3-Nitrobenzaldehyde [99-61-6]



Identity
3D Structure
Physicochemical data
Environmental fate
Mammal toxicology
Ecotoxicology
Metabolism
Limit values and classifications
Evaluation

Name	3-Nitrobenzaldehyde
Synonyms	
Name in Chemical Abstracts	Benzaldehyde, 3-nitro-
CAS No	99-61-6
EINECS No	202-772-6
Molecular formula	$C_7H_5NO_3$
Molecular mass	151.12
SMILES code	O=Cc1cc(N(=O)=O)ccc1

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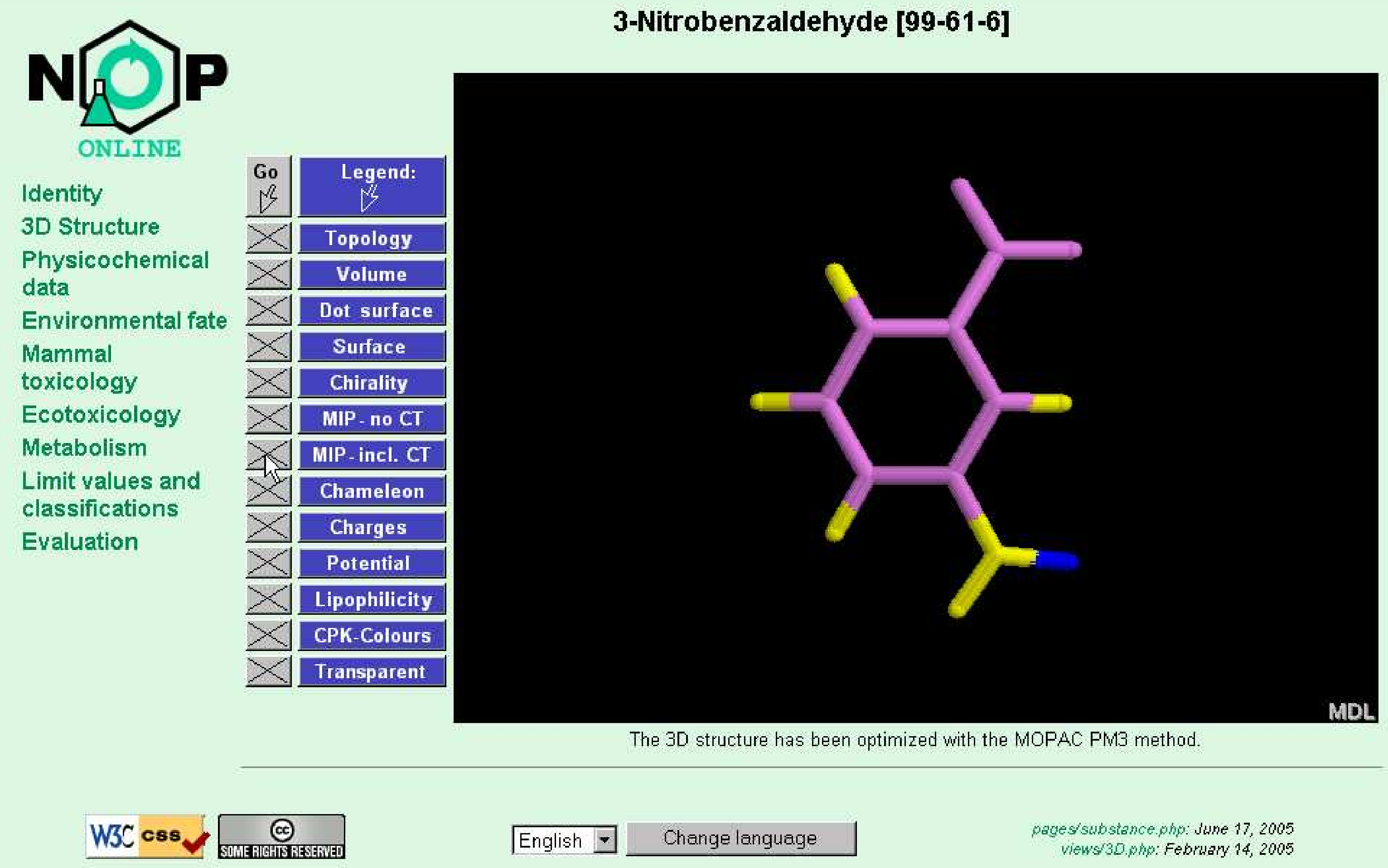
3D molecular interaction potentials



Version control

[nop] / www / pages / substance.php   Project Root: nop Go

View of /www/pages/substance.php

Parent Directory | Revision Log

Revision: **201** - (**download**) (**as text**)
Fri Jun 17 15:30:45 2005 UTC (14 hours, 49 minutes ago) by *ranke*
File size: 4005 byte(s)

Some cosmetics and a better explanation of the NOP project in the acronym explanation page.

```
<?php
if (!$_GET["chent_id"]) $chent_id= "1"; else $chent_id = $_GET["chent_id"];
if (!$_GET["view"]) $view = "identity"; else $view = $_GET["view"];

if (!$subview)
{
    switch ($view)
    {
        case "evaluation":
                $subview = "indicators";
                break;
    }
}
```

Environmental fate

ONLINE

- Identity
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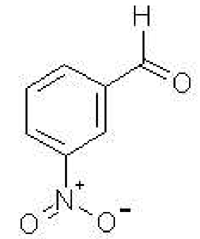
3-Nitrobenzaldehyde [99-61-6]



	value	comment	source
Water solubility	1630 mg/L at 25 °C		EPIWIN 3.10
Octanol water distribution coefficient log Kow	1.47 at room temperature		EPIWIN 3.10
Octanol water distribution coefficient log Kow	1.53 at room temperature	calculated	EPIWIN 3.10
Soil adsorption coefficient log Koc	1.58	calculated	EPIWIN 3.10
Henry constant	0.0538 Pa·m^3/mol at 25 °C	calculated	EPIWIN 3.10

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Metabolism

3-Nitrobenzaldehyde [99-61-6]

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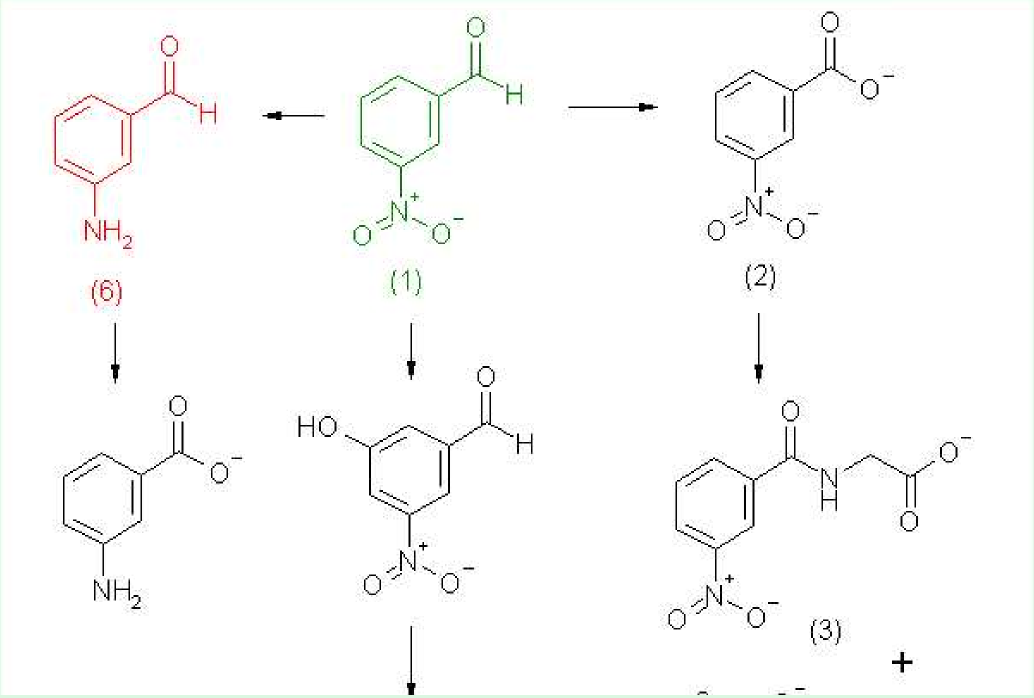
Theoretical prediction: In mammals an aldehyde dehydrogenase oxidizes 3-nitrobenzaldehyde (1) to 3-nitrobenzoic acid (2). This metabolite can be excreted as a glycine conjugate (3) or as glucuronic acid ester (4). Also 3-nitrobenzaldehyde (1) can be metabolized by cytochrome P450 with hydroxylation of the aromatic ring and subsequent oxidation to the corresponding benzoic acid derivates (5). A possible reduction to the aromatic amine (3-aminobenzaldehyde (6)) which generates toxic intermediates is probably less important, but cannot be excluded totally.



Conclusions

Status

- First adoptions in lab courses in Germany

Status

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- English version useable, but not complete

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Your contributions are welcome!

Acknowledgements

- Deutsche Bundesstiftung Umwelt

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- Consortium INCA

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- Consortium INCA
- All contributors

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- All contributors
- US EPA and American Chemical Society

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