



## Short Introduction to the Contents of the NOP

### Texts and background information

The NOP Database offers information on many topics of modern organic chemical education in the form of brief texts. These texts are to be used for independent studies, or as a basis of lectures. The following categories offer articles on the given subjects [Sustainability](#), [NOP - How?](#) and [Techniques](#):

- Sustainability
- Laws and regulations
- Evaluation procedure for chemical substances, reactions, and wastes
- Physical, chemical, toxicological, and ecotoxicological descriptors
- Information sources for the topic areas of environmental protection and workplace safety
- Environmental management (e.g. waste disposal)
- Contents and compilation of an ecobalance
- Application of energy in chemical reactions (e.g. by microwave radiation)
- Energy measurement and energy indices
- Optimization of reactions and minimization of wastes.

An approach to classical lab-course related topics like

- Work methods in the laboratory,
- Chromatography and
- Spectroscopy

is found in compilations of current information sources in English language, which may be found in most scientific libraries, and which are used in many lab courses.



The [Glossary](#), which features a search function, provides short definitions of terms as well as links to more in-depth texts, e.g. on energy efficiency, heat of reaction, or on toxic trace pollutants like dioxins or polychlorinated biphenyls (PCB).

## Characteristic data of chemicals

Only a person who is aware of what is already known about properties and effects of a chemical is able to perform sustainable experiments with chemical substances. Thus, if you select the menu entry "substances" for a specific experiment, you will find the data availability for each chemical shown in graphical form. You can see at a glance how much information on properties and effects of each chemical can be currently retrieved from literature. The menu heading effect factors provides an overview on the hazard potential (to human health) of all chemicals used or produced in the experiment. After a click on the name of a chemical in the list you can find under the heading limit values/ classifications, if this substance is listed in the (German) MAK-Werte Liste (List of TLV values) (occupational health and safety). Also if the German Umweltbundesamt (Federal Environmental Agency for People and the Environment) has classified this substance as a water-polluting chemical with a water pollution class you also find this information here (environmental protection). A direct link to property and effect data on chemicals without using the lab experiment pages is provided by the substances field on the NOP entry page. Specific substances can be located by a search function. A link list to internet pages and data bases can be found here that we thought useful for an independent search on properties and effects of chemicals.

For the chemicals in the NOP database physico-chemical, toxicological and ecotoxicological data can be displayed directly. Thus the foundations on which the classification of a substance (risk phrases, safety phrases, TLV and water pollution class) is based become understandable. Classifications and the German "Betriebsanweisungen" are given accordingly. But only few substances in the NOP have complete data sets at the moment. Sometimes the necessary experimental research has not yet been done and sometimes not all data could be found in the public literature. In these cases you only find the headings identity, 3-D structure and limit values/ classifications for the substance in question. This shall encourage the users of the



NOP to start an independent search for more data. As a starting point we provide under the heading identity the CAS number of the substance. Additional hints for a successful search can be found in the paragraph on [Hazard assessment for chemical substances](#) under [NOP – How?](#)

## Lab experiments

Like in all other lab courses the experiments are the central part of the NOP. The field [Experiments](#) leads to the starting page, where specific experiments can be chosen according to different criteria. These criteria include substance classes, reaction types, work methods and degree of difficulty. You can also retrieve a list of all (about 75) available experiments here. The NOP collection comprises two groups of lab experiments: The experiments of the NOP teaching module (Lehrmodul) have been extensively optimized, analyzed and assessed. These lab experiments are meant as standards and exemplify how chemical reactions can be optimized and assessed even in an educational context. The titles of all NOP teaching module experiments are shown on a grey background for easy identification. For all other experiments data necessary for safely performing the experiments are provided as well as a complete analysis of the products, but they have not been extensively optimized and assessed. Students and teachers are thus given the opportunity to optimize these in their own projects.

For each experiment the overview page shows the reaction equation, the reaction type, the substance classes involved and the most important work methods. Some of the reactions may be conducted in different ways or variants, e.g. with classical laboratory equipment or alternatively using a microwave oven. If an alternative reaction variant is available, its number is shown below the current NOP-No. This number is directly linked to the corresponding experiment.

The page for the instructions shows commented synthesis instructions for up to three batch sizes for the experiments in the NOP teaching module, typically 10 and 100 mmol. The procedure to perform the reaction, the purification and the recycling of substances is addressed in this section. Also mentioned are the average time for the experiment, possible points of interruption and waste management. The comments illustrate the techniques used and the chemicals. For all experiments a synthesis instruction for all batch sizes is provided as a pdf file, along with analytical data, additional comments, short waste management



procedures and a complete list of the substances required. The pdf document may be printed and used as an immediate instruction in the lab, where computers with internet access are often lacking.

In the operating scheme which is provided for all experiments the total work flow is shown together with all materials' flow. The graphical operating scheme also is a good overview for finding potential optimization targets, e.g. in the recycling or processing of wastes or the identification of by-products.

The menu item "substances" has already been discussed in detail. The next menu item "equipment" lists all necessary laboratory equipment for the experiment with photos to help student beginners and especially foreign students to identify new or unknown lab equipment. The menu item "evaluation" compiles the most important indices for the reaction as yield, atom economy, mass efficiency, the masses of the input substances and the masses of the products.

Some of the experiments also have an evaluation text, which tries to integrate different criteria for the assessment, e.g. toxicity of the substances used or produced, yield, the amount of wastes or energy used etc. for a more complete sustainability assessment. An approximate assessment is also indicated by the traffic light symbols: The green light marks experiments where mass efficiency and energy efficiency is quite good and the use of dangerous substances is minimal. The yellow light is given for experiments with some risks for human health and/or the environment, and that therefore must be conducted with the appropriate caution and safety measures. The red light warns for problematic aspects of the experiment, which turned up during the hazard assessment. For these experiments extensive safety precautions have to be taken and also these experiments should be optimized - or even replaced by less dangerous ones. If the traffic light symbol shows a question mark, then the experiment is usable according to the criteria of the NOP (e.g. no highly toxic, or ecotoxic or persistent substances are used or produced in the experiment, the mass efficiency and the energy efficiency is optimizable and it illustrates an important reaction type in organic chemistry). A potential risk for human health or the environment has been assessed by the evaluation of data availability and the classification according to effect factors, risk phrases, safety phrases, TLV values and water pollution classes. For substances that are not already part of the NOP teaching module, additional data should be searched by the students. This way they can train their skills in assessing the hazard potential of chemicals themselves. All



experiments with the red light and those without complete evaluation can be used in the lab course training, if the necessary safety measures are applied.

The menu item "analytics" shows in most cases a chromatogram (GC or HPLC) of the crude and the purified product together with the chromatographic data. For spectroscopic identification the proton nuclear magnetic resonance spectrum and the  $^{13}\text{C}$  NMR are given as well as the infrared spectrum. These spectra are also usually provided for the crude product as well as for the purified product. The spectra of the NOP teaching module experiments are mostly also given in an interactive form, side by side with a 3D model of the product.

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