chemexec

v1.0

March 06. 2011

Clemens Niederberger

Contents

1 Licence

chemexec v1.0 underlies the LaTeX Project Public License Version 1.3 or any later version.
(`http://www.latex-project.org/lppl.txt`)

2 About

The chemexec package provides some environments and commands I needed when I created exercise sheets and other teaching material. There is a `definition` environment, the `beispiel` environment for examples ('beispiel' is german for example) and lots of other little commands I found useful.
For the exercise sheets I especially wanted an easy way to create numbered exercises and a flexible way to print out the corresponding solutions (see section 7).
chemexec also replaces `echem.sty` for OCHEM[1].

3 New in version v1.0

chemexec lost the commands `\lw`, `\lwbar`, `\atomconnect` and the `Schema` environment, because Lewis formulæ can more easily be created with the 'ChemFig' package and several other packages (e. g. myChemistry) also provide reaction scheme environments.
chemexec now nicely works with `pdflatex`, since there are no more commands using pstricks. I used Ti*k*Z instead.

4 Package options

You can load chemexec with different options:

- The `chapter` option changes the counter of the exercises and solutions (see section 7) and of the `beispiel` environment (see section 6.1).
- The `color=<color>` changes the color of the numbers with which the exercises ans solutions are numbered. It also changes the color of the lines bordering the `beispiel` environments and the color of the title of the `definition` environment.
  Default color is `dunkelblau` defined by
  `\xdefinecolor{dunkelblau}{rgb}{0,0.33,0.62}`.
- The `english` option changes the german titles into english ones: "Aufgabe" ↔ "Exercise", "Lösung" ↔ "Solution", "Beispiel" ↔ "Example" and "Exkurs" ↔ "Excursus".
- The `exercise` option activates the commands for creating exercises and the corresponding solutions.
- The `exersize=<fontsize>` changes the fontsize of the titles of the exercises and their solutions.
- The `shade=<boolean>` changes the layout of the `definition` environment. Default is `false`.

[1] by Ingo Klöckl http://tug.ctan.org/tex-archive/support/ochem/

- The option `shadecolor=<color>` changes the background color of the `definition` environment if the option `shade=true` is used. Default is `pink!50`.
- The `numcolor=<color>` changes the color of the numbers numbering the exercises and solutions.

5 New commands

5.1 Maths

Just some small macros I found useful:

- `\vek{}` writing vectors with an arrow: `\vek{a}, \vek{A}` $\vec{a}$, $\vec{A}$.
- `$\abs{}$` absolute value: `\abs{\vek{a}}, \abs{-\frac{i}{2}}` $|\vec{a}|$, $\left|-\frac{i}{2}\right|$.

These commands can be used both in math mode and in text mode.

5.2 Chemistry

More macros I found useful. All chemistry commands can be used both in math mode and in text mode.

5.2.1 Particles ans charges

- `\el` electron: $e^{\ominus}$
- `\prt` proton: $p^{\oplus}$
- `\ntr` neutron: n^{0}
- `\Hpl` proton: $\mathrm{H}^{\oplus}$
- `\Hyd` hydroxide: $\mathrm{OH}^{\ominus}$
- `\ox{}{}` oxidation states
  `Ca\ox{-1}{F}$_2$` $\mathrm{Ca}\overset{-1}{\mathrm{F}}_2$;
  the first argument is the oxidation state, the second one the element.
- `\om` and `\op` charges $^{\ominus}$ und $^{\oplus}$.
  These commands have an optional argument for the number of charges:
  `Ca\op[2]` $\mathrm{Ca}^{2\oplus}$, `\phosphat\om[3]` $\mathrm{PO_4}^{3\ominus}$.

5.2.2 Stereo descriptors

Some descriptors to make it easier writing the correct IUPAC name:

- `\Rcip` and `\Scip`, rectus and sinister: *(R) (S)*
- `\Dfi` and `\Lfi`, dexter and laevus: D L
- `\E` and `\Z`, opposite (german: entgegen) and together (german: zusammen): *(E) (Z)*
- `\rconf` and `\sconf` R/S configuration: (R) and (S). Both commands have an optional argument changing the letter: `\rconf[]` `\sconf[A]` ( ) (A)

5.2.3 Anions

I don't use them anymore since I found the 'mhchem' package, but they're defined anyway:

- `\nitrat` : NO_3
- `\nitrit` : NO_2
- `\sulfat` : SO_4
- `\sulfit` : SO_3
- `\phosphat` : PO_4
- `\phosphit` : PO_3
- `\carbonat` : CO_3

5.2.4 Compatibility with 'mhchem'

You can use all chemistry commands in the formula commands of the 'mhchem' package[1] like `\ce{}`. 'mhchem' is loaded automatically by chemexec if it is installed. If you want to load 'mhchem' with other options than `version=3` you need to load it seperately *before* loading chemexec.

```
\ce{2␣\ox{0}{Ca}␣+␣\ox{0}{O}_2␣->T[{~~~REDOX~~~}]␣2Ca␣\op[2]
  ␣+␣2O␣\om[2]}
```

$$2\overset{0}{\mathrm{Ca}} + \overset{0}{\mathrm{O}}_2 \xrightarrow{\text{REDOX}} 2\,\mathrm{Ca}^{2\oplus} + 2\,\mathrm{O}^{2\ominus}$$

Please keep in mind that you need to leave the blanks before `\om`, `\op`, `\ox{}{}`. Else you might get unexpected results:`\ce{Ca\op[2]}` $\mathrm{Ca}^{\oplus}[_2]$.
Some more examples:

[1] by Martin Hensel http://www.ctan.org/tex-archive/macros/latex/contrib/mhchem/

```
\begin{align*}
 \cee{Na                    &->T[ox] Na\op{} + \el}\\
 \cee{HCl_{aq}              &<=>> H\op_{aq} + Cl\om_{aq}}\\
 \cee{H2O                   &<<=> \Hpl + \Hyd}\\
 \cee{CaCl2 + H2\sulfat{}} &-> Ca\sulfat{} v + 2 HCl}
\end{align*}
```

$$\begin{aligned}
\mathrm{Na} &\xrightarrow{\mathrm{ox}} \mathrm{Na^{\oplus}} + e^{\ominus} \\
\mathrm{HCl_{aq}} &\rightleftharpoons \mathrm{H^{\oplus}_{aq}} + \mathrm{Cl^{\ominus}_{aq}} \\
\mathrm{H_2O} &\rightleftharpoons \mathrm{H^{\oplus}} + \mathrm{OH^{\ominus}} \\
\mathrm{CaCl_2} + \mathrm{H_2SO_4} &\longrightarrow \mathrm{CaSO_4}\downarrow + 2\,\mathrm{HCl}
\end{aligned}$$

5.2.5 Commands for 'mhchem'

chemexec also provides some commands for numbered and centered reactions created by 'mhchem'.

```
Reaction with a number:
\reaction{2 H2 + O2 -> 2 H2O}%
Reaction without a number:
\reaction*{2 CO + O2 -> 2 CO2}
More reactions at once, aligned:
\reactions{Cl_2 &-> 2 Cl. \\ Cl. + CH4 &-> HCl + {}.CH3}
```

Reaction with a number:

$$2\,\mathrm{H_2} + \mathrm{O_2} \longrightarrow 2\,\mathrm{H_2O} \tag{R 1}$$

Reaction without a number:

$$2\,\mathrm{CO} + \mathrm{O_2} \longrightarrow 2\,\mathrm{CO_2}$$

More reactions at once, aligned:

$$\begin{aligned}
\mathrm{Cl_2} &\longrightarrow 2\,\mathrm{Cl}\cdot && \text{(R 2)} \\
\mathrm{Cl}\cdot + \mathrm{CH_4} &\longrightarrow \mathrm{HCl} + \cdot\mathrm{CH_3} && \text{(R 3)}
\end{aligned}$$

6 New environments

6.1 The `beispiel` environment - creating examples

The `beispiel` environment is an environment for examples. Examples automatically are numbered and placed between two lines. The fontsize of the examples is `\small`.

```
\begin{beispiel}
 an example
\end{beispiel}
```

Example 1:
an example

If you want to give two or more examples in between the same two lines, you can use `\bsp`:

```
\begin{beispiel}
 first example
 \bsp
 second one
\end{beispiel}
```

Example 2:
first example
Example 3:
second one

6.1.1 The options `color`, `linecolor` & `english`

The `linecolor=<color>` option changes the color of the lines:

```
% preamble:
\usepackage[linecolor={rgb:red,4;green,6}]{chemexec}
% in the document:
\begin{beispiel}
 green lines through package option
\end{beispiel}
```

folgenden Output:

Example 4:
green lines through package option

The option `color=<color>` also changes the color of the lines (but also changes the color of other things,too).
By using the key `linecolor=<color>` you can change the color of a single example:

```
\begin{beispiel}[linecolor=purple]
 the lonely purple one
\end{beispiel}
```

folgenden Output:

Example 5:
the lonely purple one

The `english` option translates "Beispiel" into "Example".

6.1.2 Not numbered examples

If you don't like the numbering you can redefine the counter as usual.

```
\renewcommand{\thebeispiel}{}
\begin{beispiel}
 now without counter
\end{beispiel}
```

Example
now without counter

```
\renewcommand{\thebeispiel}{\alph{beispiel})}
\begin{beispiel}
 or alphabetically \ldots
\end{beispiel}
```

Example g)
or alphabetically ...

6.2 The `definition` environment

The `definition` environment creates a box with a colored title:

```
\begin{definition}
 The absolut value of a vector in $\mathbb{R}^3$ is
 \begin{equation}
  \abs{\vek{a}}=\sqrt{a_x^2+a_y^2+a_z^2}
 \end{equation}
\end{definition}
```

DEFINITION The absolut value of a vector in $\mathbb{R}^3$ is

$$|\vec{a}| = \sqrt{a_x^2 + a_y^2 + a_z^2} \tag{1}$$

6.2.1 The options `shade`, `shadecolor` & `color`

With the key `shade=<boolean>` you can change the layout:

```
\begin{definition}[shade=true]
 The absolut value of a vector in $\mathbb{R}^3$ is
 \begin{equation}
  \abs{\vek{a}}=\sqrt{a_x^2+a_y^2+a_z^2}
 \end{equation}
\end{definition}
```

DEFINITION The absolut value of a vector in $\mathbb{R}^3$ is:

$$|\vec{a}| = \sqrt{a_x^2 + a_y^2 + a_z^2} \tag{2}$$

By using the keys `shadecolor=<color>` und `color=<color>` you can customize the environment:

```
\begin{definition}[shade=true,shadecolor=green!15,color=black]
 The absolut value of a vector in $\mathbb{R}^3$ is
 \begin{equation}
  \abs{\vek{a}}=\sqrt{a_x^2+a_y^2+a_z^2}
 \end{equation}
\end{definition}
```

DEFINITION The absolut value of a vector in $\mathbb{R}^3$ is:

$$|\vec{a}| = \sqrt{a_x^2 + a_y^2 + a_z^2} \tag{3}$$

You can use all of these keys as package options as well. This way, you can change the layout of every `definition` environment at once. Please keep in mind, that in this case `color=<color>` also has effects on other commands and environments.

```
% preamble:
\usepackage[shade=true,shadecolor=yellow!15]{chemexec}
% in the document:
\begin{definition}
 The absolut value of a vector in $\mathbb{R}^3$ is
 \begin{equation}
  \abs{\vek{a}}=\sqrt{a_x^2+a_y^2+a_z^2}
 \end{equation}
\end{definition}
```

DEFINITION The absolut value of a vector in $\mathbb{R}^3$ is:

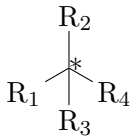
$$|\vec{a}| = \sqrt{a_x^2 + a_y^2 + a_z^2} \tag{4}$$

6.2.2 The `defformel` environment

There is an additional environment, which only creates a white box. It has an optional argument for the width of the box.

```
\begin{definition}[shade=true]
 A carbon atom with four different substituents is called \textbf{
    asymmetric}. Asymmetric carbon atoms often are labelled with a \
    textasteriskcentered.
 \begin{defformel}[.5\textwidth]
  \setatomsep{1.8em}
  \chemfig{R_1-[:30](-[2]R|_2)(-[6]R|_3)(-[:30,.15,,,white]{\text{\
      textasteriskcentered}})-[:-30]R_4}
 \end{defformel}
\end{definition}
```

DEFINITION A carbon atom with four different substituents is called **asymmetric**. Asymmetric carbon atoms often are labelled with a $*$.



6.3 The `exkurs` environment

The `exkurs` environment is used to visually highlight an excursus (in a book or longer text) and produce an entry in the table of contents.

```
\begin{exkurs}[options]{title}
 ...
\end{exkurs}
```

You have two options: the `toc=<toclevel>` option with `section` as default and the `color=<color>` option.

```
\begin{exkurs}[color=-yellow]{Lorem ipsum}
 Lorem ipsum dolor sit amet, consectetuer adipiscing elit, sed diam
    nonummy nibh euismod tincidunt ut laoreet dolore magna aliquam erat
    volutpat. ...
\end{exkurs}
```

EXCURSUS: Lorem ipsum

Lorem ipsum dolor sit amet, consectetuer adipiscing elit, sed diam nonummy nibh euismod tincidunt ut laoreet dolore magna aliquam erat volutpat. Ut wisi enim ad minim veniam, quis nostrud exerci tation ullamcorper suscipit lobortis nisl ut aliquip ex ea commodo consequat. Duis autem vel eum iriure dolor in hendrerit in vulputate velit esse molestie consequat, vel illum dolore eu feugiat nulla facilisis at vero eros et accumsan et iusto odio dignissim qui blandit praesent luptatum zuril delenit augue duis dolore te feugait nulla facilisi.

If you use color=<color> it also chages the color in other environments. The package option english changes the german caption "Exkurs" into "Excursus".

7 The option exercise: numbered exercises/solutions

The main part of chemexec provides the commands for exercises and their solutions, which can be activated by the package option exercise. Exercises have "Aufgabe" or "Exercise", respectively, as default title, which can be changed with the argument.

```
\aufgabe{<title>}
```

For creating the solutions to the exercises, there are three commands:

```
\loesung[<title>]{<solution>} % remember the solution
\doloesung % writing the solutions sectionwise
\makeloesung % writing all solutions
```

The first command \loesung{} is used, to write the solution of an exercise *directly after the exercise*. The second command \doloesung writes all the solutions gathered in the actual section by the \loesung{} commands. Since sections reset the counter of the exercises and \doloesung resets gathering of the solutions, you should use \doloesung at the end of a section. Otherwise, the numbers of the solutions might not be the numbers of the corresponding exercises anymore. If you're creating a document which has chapters, you should keep in mind, that \doloesung should be used at the end of a chapter, if you had exercises in that chapter. Instead of \doloesung, you can use \makeloesung once after *all* exercises and solutions are set to write all the solutions.

7.1 Options

With the exersize=<fontsize> option you can change the fontsize of the exercises' and solutions' titles. Possible values are the usual ones: tiny, scriptsize, footnotesize, small, normalsize, large, Large, LARGE, huge and Huge.
Default font size is normalsize.
The numcolor=<color> package option changes the color of the numbers with which the exercises are numbered. The english package option translates "Aufgabe" into "Exercise" and "Lösung" into "Solution".
In the default behaviour chemexec resets the numbers of the exercises with each new \section. If you use the chapter package option, the counter is reset with each new \chapter.

7.2 The alphlist environment

The alphlist environment creates a list similar to the enumerate environment, but counts the items with a), b) etc.

```
\begin{alphlist}
 \item first item
 \item second item
\end{alphlist}
```

a) first item

b) second item

7.3 Example

In the following example you see the `\aufgabe`, `\loesung` and `doloesung` commands in action.

```
% preamble:
\usepackage[exercise,exersize=large]{chemexec}
% Im Dokument:
\par{\Large\bfseries\noindent Exercises}
\aufgabe{}
 Write down the protolysis reactions of phosphoric acid.\loesung{\ce{
     H3PO4 <=> \Hpl{} + H2PO4\om{} <=> 2\Hpl{} + HPO4 \om[2]{} <=> 3\Hpl{}
      + PO4 \om[3]{}}}
\aufgabe{Oxidation states}
 Which oxidation state has nitrogen in thze following compounds: ammonia,
      nitric oxide, nitrogen dioxide, nitric acid?\loesung[Oxidation
     states]{
 \ce{ \ox{-3}{N} H3}, \ce{ \ox{+2}{N} O}, \ce{ \ox{+4}{N} O2}, \ce{H \ox
     {+5}{N} O3}}
\aufgabe{Nomenclature}
 Name the molecules:\\\setatomsep{1.4em}
 \begin{inparaenum}[a)]
  \item\chemfig{-[::30](=[::60]O)-[::-60]OH}
  \item\chemfig{-[::30](=[::60]O)-[::-60]O-[::60]-[::-60]}
  \item\chemfig{HO-[::-30](=[::-60]O)-[::60]-[::-60]-[::60](=[::60]O)
      -[::-60]OH}
 \end{inparaenum}
\loesung[Nomenclature]{
 \begin{inparaenum}[a)]
  \item ethanoic acid
  \item ethyl ethanoate
  \item butanedioic acid
 \end{inparaenum}
}
\aufgabe{}
 Sketch the skeletal formula of glycerol. Also give the IUPAC name.
\loesung{\chemname{\chemfig{HO-[::-30]-[::60](-[::60]OH)-[::-60]-[::60]OH
    }}{1,2,3-Propantriol}}
\vspace{\baselineskip}
\par{\Large\bfseries\noindent Solutions}
\doloesung
```

Exercises

1. Exercise

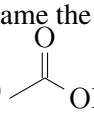
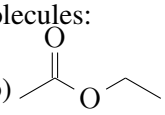
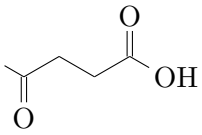
Write down the protolysis reactions of phosphoric acid.

2. Oxidation states

Which oxidation state has nitrogen in thze following compounds: ammonia, nitric oxide, nitrogen dioxide, nitric acid?

3. Nomenclature

Name the molecules:

a)  b)  c) 

4. Exercise

Sketch the skeletal formula of glycerol. Also give the IUPAC name.

Solutions

1. Solution

$$H_3PO_4 \rightleftharpoons H^{\oplus} + H_2PO_4^{\ominus} \rightleftharpoons 2\,H^{\oplus} + HPO_4^{2\ominus} \rightleftharpoons 3\,H^{\oplus} + PO_4^{3\ominus}$$

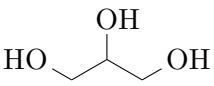
2. Oxidation states

$\overset{-3}{N}H_3$, $\overset{+2}{N}O$, $\overset{+4}{N}O_2$, $H\overset{+5}{N}O_3$

3. Nomenclature

a) ethanoic acid b) ethyl ethanoate c) butanedioic acid

4. Solution



propan-1,2,3-triol

7.4 Bugs?

It is very likely, that either `\doloesung` or `\makeloesung` or both have bugs. If you detect any, please let me know.

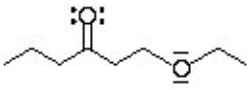
8 Replacement for echem.sty

The echem.sty is part of Ingo Klöckls OCHEM[1]. It enables the lewis representation of electrons. Additionally echem.sty provides the commands \sbond und \dbond with which you can typeset a single or a double bond in normal text. Both commands are defined in the 'mhchem' package as well-

- 'mhchem':
  - \ce{F\sbond F}: F–F
  - \ce{O\dbond O}: O=O
- 'echem':
  - F\sbond F: F·F
  - O\dbond O: O=O

To avoid conflicts with 'mhchem' besides these two commands and the commands \2 and \3 chemexec has the same functionality as echem.sty. So it can be used instead of echem.sty in OCHEM's chemspecial environment.

```
% preamble
\usepackage{ochem,chemexec}
% in the document:
\begin{chemspecial}
 package("chemexec")
\end{chemspecial}
\begin{chemistry}
 formula(L,R){
   bond(30;-30;30)
   branch { bond(90,=C)
            atom("\vdd{O}O\vdd{O}");
          }
   bond(-30;30;-30)
   atom("\hdl[\echhbar]{O}\hdu[\echhbar]{O}O",L,R)
   bond(30;-30)
 }
\end{chemistry}
```



9 Epilogue

I tried using real chemical reactions but I didn't make sure, that they all make sense chemically. So you shouldn't trust the examples in respect to chemistry but rather take a look into a real chemistry teaching book.
I apologize for any bad or wrong English. I hope you understood the documention anyway.

[1] http://tug.ctan.org/tex-archive/support/ochem/