the chemmacros bundle

v4.0 2013/07/06

packages **chemmacros** (v4.0), **chemformula** (v4.0), **ghsystem** (v4.0) and **chemgreek** (v0.1a)

documentation for the **chemformula** package

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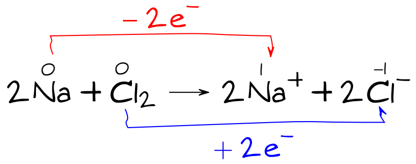
English documentation



$$2\,\overset{0}{Na} + \overset{0}{Cl}_2 \longrightarrow 2\,\overset{I}{Na}^{+} + 2\,\overset{-I}{Cl}^{-}$$

Contents

1 Introduction

Probably every chemist using LaTeX 2ε is aware of the great mhchem[1] package by Martin Hensel. There have always been some difficulties intertwining it with CHEMMACROS, though. Also, some other minor points in mhchem always bothered me, but they hardly seemed enough for a new package. They weren't even enough for a feature request to the mhchem author. The challenge and the fun of creating a new package and the wish for a highly customizable alternative led to CHEMFORMULA after all.

CHEMFORMULA works very similar to mhchem but is more strict as to how compounds, stoichiometric factors and arrows are input. In the same time CHEMFORMULA offers *many* possibilities to customize the output.

Introduced in version 4.0

Since version 4.0, the CHEMFORMULA package can be used independently from CHEMMACROS. This means that if you say

```
\usepackage{chemformula}
```

then CHEMMACROS will not be loaded. The CHEMMACROS package, however, *will* load CHEMFORMULA.

2 Licence and Requirements

Permission is granted to copy, distribute and/or modify this software under the terms of the LaTeX project public license (lppl) version 1.3 or later (`http://www.latex-project.org/lppl.txt`). The package has the status "maintained."

The CHEMFORMULA package needs and thus loads the packages expl3 (from the l3kernel[2]), xparse, l3keys2e and xfrac (from the l3packages[3]), tikz,[4] amsmath,[5] nicefrac and scrlfile (from the KOMA-Script[6] bundle).

3 Setup

All of CHEMFORMULA's options belong to CHEMMACROS' module `chemformula`. This means they can be setup with

```
\chemsetup[chemformula]{<options>} or
\chemsetup{chemformula/<option1>,chemformula/<option2>}
```

---

[1] on CTAN: mhchem [2] on CTAN: l3kernel [3] on CTAN: l3packages [4] on CTAN: pgf [5] on CTAN: amsmath [6] on CTAN: koma-script

However, if you're using CHEMFORMULA as a standalone package the command `\chemsetup` is not available. This is why CHEMFORMULA also has its own setup command:

```
\setchemformula{<options>}
```

4 The Basic Principle

CHEMFORMULA offers one main command.

```
\ch[<options>]{<input>}
```

The usage will seem very familiar to you if you're familiar with mhchem:

```
\ch{H2O} \\
\ch{Sb2O3} \\
\ch{H+} \\
\ch{CrO4^2-} \\
\ch{AgCl2-} \\
\ch{[AgCl2]-} \\
\ch{Y^{99}+} \\
\ch{Y^{99+}} \\
\ch{H2_{(aq)}} \\
\ch{NO3-} \\
\ch{(NH4)2S} \\
\ch{^{227}_{90}Th+} \\
$V_{\ch{H2O}}$ \\
\ch{Ce^{IV}} \\
\ch{KCr(SO4)2 * 12 H2O}
```

H_2O
Sb_2O_3
H^+
CrO_4^{2-}
$AgCl_2^-$
$[AgCl_2]^-$
Y^{99+}
Y^{99+}
$H_{2(aq)}$
NO_3^-
$(NH_4)_2S$
${}^{227}_{90}Th^+$
V_{H_2O}
Ce^{IV}
$KCr(SO_4)_2 \cdot 12\,H_2O$

However, there are differences. The most notable one: CHEMFORMULA distinguishes between different types of input. These different parts *have* to be separated with blanks:

```
\ch{part1 part2 part3 part4}
```

A blank in the input *never* is a blank in the output. This role of the blank strictly holds and disregarding it can have unexpected results and even lead to errors.

Another notable difference: CHEMFORMULA tries to avoid math mode whenever possible:

```
\ch{A + B ->[a] C} \\
\ce{A + B ->[a] C}
```

$\mathrm{A} + \mathrm{B} \xrightarrow{\mathrm{a}} \mathrm{C}$
$A + B \xrightarrow{a} C$

This means that `\ch{2H2O}` is recognized as a *single* part, which in this case is recognized as a compound.

```
\ch{2H2O} \\
\ch{2 H2O}
```

${}_2H_2O$
$2\,H_2O$

This also means, that a part cannot contain a blank since this will automatically divide it into two parts. If you need an extra blank in the output you need to use `~`. However, since commands in most cases gobble a space after them a input like `\ch{\command ABC}` will be treated as a single part. If you want or need to divide them you need to add an empty group: `\ch{\command{} ABC}`. The different input types are described in the following sections.

There are some options to customize the output of the `\ch` command. They can either be applied locally using the optional argument or can be set globally using the setup command. All options of CHEMFORMULA belong to the module `chemformula` and can be set in different ways:

`\chemsetup[chemformula]{<options>}` (when loaded via CHEMMACROS)

`\chemsetup{chemformula/<options>}` (when loaded via CHEMMACROS)

`\setchemformula{<options>}` (independent from CHEMMACROS)

5 Stoichiometric Factors

A stoichiometric factor may only contain of numbers and the signs `.,_/()`

```
\ch{2} \\
\ch{12}

% decimals:
\ch{.5} \\
\ch{5,75}

% fractions:
\ch{3/2} \\
\ch{1_1/2}

% ``iupac'':
\ch{(1/2)}
```

2
12
0.5
5.75
$\frac{3}{2}$
$1\frac{1}{2}$
(1/2)

As you can see if you input decimal numbers a missing leading zero is added.
You have to be a little bit careful with the right syntax but I believe it is rather intuitive.

```
this won't work but will result in an error: \ch{1/1_1}
```

If stoichiometric factors are enclosed with parentheses the fractions are not recognized and missing leading zeros are not added. What's inside the parentheses is typeset as is.

```
\ch{(1/2) H2O} \ch{1/2 H2O} \ch{0.5 H2O}
```

(1/2) H_2O $\frac{1}{2}$ H_2O 0.5 H_2O

You can find many examples like the following for stoichiometric factors in parentheses in the IUPAC Green Book [Coh+08]:

$$(1/5)\,\mathrm{KMn^{VII}O_4} + (8/5)\,\mathrm{HCl} \quad = \quad (1/5)\,\mathrm{Mn^{II}Cl_2} + (1/2)\,\mathrm{Cl_2} + (1/5)\,\mathrm{KCl} + (4/5)\,\mathrm{H_2O}$$

There are a few possibilities to customize the output.

`decimal-marker = <marker>` Default: `.`

The symbol to indicate the decimal.

`frac-style = math|xfrac|nicefrac` Default: `math`

Determines how fractions are displayed.

`stoich-space = <skip>` Default: `.1667em plus .0333em minus .0117em`

The space that is placed after the stoichiometric factor. A rubber length.

`stoich-paren-parse = true|false` Default: `false`

If set to true stoichiometric factors enclosed by parentheses also are parsed.

```
\ch[decimal-marker={,}]{3.5} \ch[decimal-marker={$\cdot$}]{3,5}
```

3,5 3·5

The option `frac-style = xfrac` uses the `\sfrac` command of the xfrac package. The output strongly depends on the font you use.

```
\ch[frac-style=xfrac]{3/2} \ch[frac-style=xfrac]{1_1/2}
```

$^{3}/_{2}$ $1^{1}/_{2}$

CHEMFORMULA defines the instance `formula-text-frac` which you can redefine to your needs. See the xfrac documentation for further information. The default definition is this:

```
\DeclareInstance{xfrac}{chemformula-text-frac}{text}
 {
   slash-left-kern  = -.15em ,
   slash-right-kern = -.15em
 }
```

This document uses the font Linux Libertine O and the following definition:

```
\DeclareInstance{xfrac}{chemformula-text-frac}{text}
 {
   scale-factor        = 1 ,
   denominator-bot-sep = -.2ex ,
   denominator-format  = \scriptsize #1 ,
   numerator-top-sep   = -.2ex ,
   numerator-format    = \scriptsize #1 ,
   slash-right-kern    = .05em ,
   slash-left-kern     = .05em
 }
```

The option `frac-style = nicefrac` uses the `\nicefrac` command of the nicefrac package.

```
\ch[frac-style=nicefrac]{3/2} \ch[frac-style=nicefrac]{1_1/2}
```

$^{3}/_{2}$ $1^{1}/_{2}$

The option `stoich-space` allows you to customize the space between stoichiometric factor and the group following after it.

```
\ch{2 H2O} \\
\ch[stoich-space=.3em]{2 H2O}
```

$2\,H_2O$
$2\;H_2O$

6 Compounds

CHEMFORMULA determines compounds as the type that “doesn’t fit in anywhere else.” This point will become more clear when you know what the other types are.

```
\ch{H2SO4} \\
\ch{[Cu(NH3)4]^2+}
```

H_2SO_4
$[Cu(NH_3)_4]^{2+}$

6.1 Adducts

CHEMFORMULA has two identifiers which will create adducts.

`\ch{A.B}`
$A\cdot B$

`\ch{A*B}`
$A\cdot B$

```
\ch{CaSO4.H2O} \\
\ch{CaSO4*H2O}
```

$CaSO_4\cdot H_2O$
$CaSO_4\cdot H_2O$

Since numbers in a compound always are treated as subscripts (see section 6.2) you sometimes need to introduce stoichiometric factors for the right output:

```
\ch{Na3PO4*12H2O} \\
\ch{Na3PO4* 12 H2O} \\
\ch{Na3PO4 * 12 H2O}
```

$Na_3PO_4\cdot{}_{12}H_2O$
$Na_3PO_4\cdot 12\,H_2O$
$Na_3PO_4\cdot 12\,H_2O$

6.2 Subscripts

All numbers in a compound are treated as subscripts.

```
\ch{H2SO4}
```

H_2SO_4

If you want a letter to be a subscript you can use the math syntax:

```
\ch{A_nB_m}
```

$\mathrm{A_nB_m}$

The subscript recognizes groups. You can also use math inside it.

```
\ch{A_{$n$}B_{$m$}} \\
\ch{NaCl_{(aq)}}
```

$\mathrm{A}_{n}\mathrm{B}_{m}$

$\mathrm{NaCl_{(aq)}}$

6.3 Commands

Commands are allowed in a compound:

```
\ch{\textbf{A2}B3} \ch{A2\color{red}B3}
```

$\mathbf{A_2}\mathrm{B_3}$ $\mathrm{A_2}\color{red}\mathrm{B_3}$

However, if the commands demand numbers as argument, e.g., space commands or CHEMMACROS' `\ox` command the direct use will fail. This is because the numbers are treated as subscripts *before* the command expands.

```
\ch{A\hspace{2mm}B} will raise an error because \hspace sees something like
this: \hspace{$_2$mm}. Actually not at all like it but equally bad\ldots
```

See section 8.1 for a way around this.

6.4 Charges and Other Superscripts

Basics If a compound *ends* with a plus or minus sign it will be treated as charge sign and typeset as superscript. In other places a plus is treated as a triple bond and a dash will be used as a single bond, see section 6.5.

```
\ch{A+B} \ch{AB+} \\
\ch{A-B} \ch{AB-}
```

$\mathrm{A{\equiv}B}$ $\mathrm{AB^+}$

$\mathrm{A{-}B}$ $\mathrm{AB^-}$

For longer charge groups or other superscripts you can use the math syntax. It recognizes groups and you can use math inside them. Inside these groups neither `+` nor `-` are treated as bonds. If a dot `.` is inside a superscript it is treated as indicator for a radical. A `*` gives the excited state.

```
\ch{A^{x-}} \\
\ch{A^x-} \\
\ch{A^{x}-} \\
\ch{A^{$x-$}} \\
\ch{RNO2^{-.}} \\
\ch{^31H} \\
\ch{^{14}6C} \\
\ch{^{58}_{26}Fe} \\
\ch{NO^*}
```

$\mathrm{A^{x-}}$

$\mathrm{A^{x-}}$

$\mathrm{A^{x-}}$

A^{x-}

$\mathrm{RNO_2^{-\bullet}}$

$\mathrm{^{3}_{1}H}$

$\mathrm{^{14}_{6}C}$

$\mathrm{^{58}_{26}Fe}$

$\mathrm{NO^{*}}$

Ions and ion composites with more than one charge can be typeset quite as easy:

```
\ch{SO4^2-} \ch{Ca^2+ SO4^2-}
```

$\mathrm{SO_4^{2-}}$ $\mathrm{Ca^{2+}SO_4^{2-}}$

Charge Commands You don't need to use `\mch` and related commands inside `\ch`. Indeed, you *shouldn't* use them as they might mess with the subscript and superscript alignment. The CHEMMACROS option `circled` is obeyed by `\ch`.

```
\chemsetup[option]{circled=all}
\ch{H+ + OH- <=> H2O}
```

$\mathrm{H^{+} + OH^{-} \rightleftharpoons H_2O}$

Behaviour The supercripts behave differently depending on their position in a compound, if there are super- and subscripts following each other directly.

```
\ch{^33B} \ch{{}^33B} \ch{3^3B} \ch{B^3} \ch{B3^3} \\
\ch{^{23}_{123}B} \ch{{}^{23}_{123}B}  \ch{_{123}^{23}B} \ch{B^{23}} \ch{B
 _{123}^{23}} \\
\ch{^{123}_{23}B} \ch{{}^{123}_{23}B}  \ch{_{23}^{123}B} \ch{B^{123}} \ch{B
 23^{123}}
```

${}^{3}_{3}\mathrm{B}$ ${}_{3}{}^{3}\mathrm{B}$ ${}^{3}_{3}\mathrm{B}$ B^{3} B_{3}^{3}
${}^{23}_{123}\mathrm{B}$ ${}_{123}{}^{23}\mathrm{B}$ ${}^{23}_{123}\mathrm{B}$ B^{23} B_{123}^{23}
${}^{123}_{23}\mathrm{B}$ ${}_{23}{}^{123}\mathrm{B}$ ${}^{123}_{23}\mathrm{B}$ B^{123} B_{23}^{123}

- If a compound *starts* with a sub- or superscript both sub- and superscript are aligned to the *right* else to the *left*.
- If a compound *does not start* with a sub- or superscript and there is both a sub- and a superscript, the superscript is shifted additionally by a length determined from the option `charge-hshift = <dim>`, also see page 10f.

The second point follows IUPAC's recommendations:

> In writing the formula for a complex ion, spacing for charge number can be added (staggered arrangement), as well as parentheses: $\mathrm{SO_4{}^{2-}}$, $\mathrm{(SO_4)^{2-}}$ The staggered arrangement is now recommended.
> *IUPAC Green Book* [*Coh+08, p. 51*]

6.5 Bonds

6.5.1 Native Bonds

There are three kinds of what I will call "native bonds":

```
single: \ch{CH3-CH3} \\
double: \ch{CH2=CH2} \\
triple: \ch{CH+CH}
```

single: $\mathrm{CH_3{-}CH_3}$
double: $\mathrm{CH_2{=}CH_2}$
triple: $\mathrm{CH{\equiv}CH}$

Table 1: Bonds available with `\bond`.

name	appearance	aliases
`single`	$-$	`normal`, `sb`
`double`	$=$	`db`
`triple`	$\equiv$	`tp`
`dotted`	$\cdots$	`semisingle`
`deloc`	$\overset{\cdots}{-}$	`semidouble`
`tdeloc`	$\overset{\cdots}{=}$	`semitriple`
`co>`	$\rightarrow$	`coordright`
`<co`	$\leftarrow$	`coordleft`

6.5.2 Flexible Bonds

Predefined Bonds In addition to the three native bonds there are a few more which can be called by

```
\bond{<bond name>}
```

The predefined bond types are shown in table 1.

```
\ch{C\bond{sb}C\bond{db}C\bond{tp}C\bond{deloc}C\bond{tdeloc}C\bond{co>}C\bond{<
 co}C}
```

$\mathrm{C}-\mathrm{C}=\mathrm{C}\equiv\mathrm{C}\overset{\cdots}{-}\mathrm{C}\overset{\cdots}{=}\mathrm{C}\rightarrow\mathrm{C}\leftarrow\mathrm{C}$

Own Bonds CHEMFORMULA offers commands to define own bond types:

```
\DeclareChemBond{<name>}{<code>}
```

```
\RenewChemBond{<name>}{<code>}
```

```
\DeclareChemBondAlias{<new name>}{<old name>}
```

```
\ShowChemBond{<name>}
```

The usage is best described with an example. So let's see how the `single` bond and the `co>` bond are defined:

```
\DeclareChemBond{single}
  { \draw[chembond] (chemformula-bond-start) -- (chemformula-bond-end) ; }
\DeclareChemBond{coordright}
  { \draw[chembond,butt cap->] (chemformula-bond-start) -- (chemformula-
 bond-end) ; }
\DeclareChemBondAlias{co>}{coordright}
```

Two points are important: the names of the starting and the ending coordinates, `chemformula-bond-start` and `chemformula-bond-end`, and the Ti*k*Z style of the bonds `chembond`.

So, let's say you want to define a special kind of dashed bond. You could do this:

```
\usetikzlibrary{decorations.pathreplacing}
\makeatletter
\DeclareChemBond{dashed}
  {
    \draw[
      chembond,
      decorate,
      decoration={ticks,segment length=\chemformula@bondlength/10,amplitude=1.5 pt}]
      (chemformula-bond-start) -- (chemformula-bond-end) ;
  }
\makeatother
\chemsetup[chemformula]{bond-length=2ex}
\ch{C\bond{dashed}C}
```

The last example showed you another macro: `\chemformula@bondlength`. It only exists so you can use it to access the bond length as set with `bond-length` directly.

6.6 Customization

These options allow you to customize the ouptut of the compounds:

`subscript-vshift = <dim>` Default: `0pt`
Extra vertical shift of the subscripts.

`subscript-style = text|math` Default: `text`
Style that is used to typeset the subscripts.

`charge-hshift = <dim>` Default: `.25em`
Shift of superscripts when following a subscript.

`charge-vshift = <dim>` Default: `0pt`
Extra vertical shift of the superscripts.

`charge-style = text|math` Default: `text`
Style that is used to typeset the superscripts.

`adduct-space = <dim>` Default: `.1333em`
Space to the left and the right of the adduct point.

`bond-length = <dim>` Default: `.5833em`
The length of the bonds.

`bond-offset = <dim>` Default: `.07em`
Space between bond and atoms.

`bond-style = <tikz>` (initially empty)
TikZ options for the bonds.

`radical-style = <tikz>` (initially empty)
TikZ options for the radical point.

`radical-radius = <dim>` Default: `.2ex`
The radius of the radical point.

`radical-hshift = <dim>` Default: `.15em`
Horizontal shift before the radical point is drawn.

`radical-vshift = <dim>` Default: `.5ex`
Vertical shift relative to the current baseline.

`radical-space = <dim>` Default: `.15em`
Horizontal shift after the radical point is drawn.

Maybe you have noticed that charges of certain ions are shifted to the right.

```
\ch{SO4^2-} \ch{NH4+} \ch{Na+}
```

SO_4^{2-} NH_4^+ Na^+

They are shifted if they *follow* a subscript which follows IUPAC recommendations [Coh+08, p. 51]. The amount of the shift can be set with the option `charge-hshift`.

```
\ch{SO4^2-} \ch{NH4+} \ch{Na+} \\
\chemsetup[chemformula]{charge-hshift=.5ex}
\ch{SO4^2-} \ch{NH4+} \ch{Na+} \\
\chemsetup[chemformula]{charge-hshift=.5pt}
\ch{SO4^2-} \ch{NH4+} \ch{Na+}
```

SO_4^{2-} NH_4^+ Na^+
SO_4^{2-} NH_4^+ Na^+
SO_4^{2-} NH_4^+ Na^+

Despite IUPAC's recommendation CHEMFORMULA does not make fully staggered arrangements in the default setting as I find it hard to read in some cases and ugly in others. Since this is a subjective decision CHEMFORMULA not only let's you define the absolute amount of the shift but also provides a possibility for full staggered arrangements. For this you have to use `charge-hshift = full`.

```
\ch[charge-hshift=0pt]{C5H11+} \ch[charge-hshift=0pt]{SO4^2-} \\
\ch{C5H11+} \ch{SO4^2-} \\
\ch[charge-hshift=1ex]{C5H11+} \ch[charge-hshift=1ex]{SO4^2-} \\
\ch[charge-hshift=full]{C5H11+} \ch[charge-hshift=full]{SO4^2-}
```

$C_5H_{11}^+$ SO_4^{2-}
$C_5H_{11}^+$ SO_4^{2-}
$C_5H_{11}^{\,+}$ $SO_4^{\,2-}$
$C_5H_{11}{}^+$ $SO_4{}^{2-}$

If you don't want the charges to be typeset in text mode you can switch to math mode:

```
\ch{M^x+} \ch{SO4^2-} \\
\chemsetup[chemformula]{charge-style = math}
\ch{M^x+} \ch{SO4^2-}
```

$\mathrm{M}^{\mathrm{x}+}$ SO_4^{2-}
M^{x+} $\mathrm{SO}_4{}^{2-}$

The option subscript-vshift can be used to adjust the vertical shift of the subscripts:

```
\ch{H2SO4} \ch{Na3PO4} \\
\chemsetup[chemformula]{subscript-vshift=.5ex}
\ch{H2SO4} \ch{Na3PO4} \\
\chemsetup[chemformula]{subscript-vshift=-.2ex}
\ch{H2SO4} \ch{Na3PO4}
```

$\mathrm{H_2SO_4}$ $\mathrm{Na_3PO_4}$
$\mathrm{H_2SO_4}$ $\mathrm{Na_3PO_4}$
$\mathrm{H_2SO_4}$ $\mathrm{Na_3PO_4}$

You can choose the mode subscripts are typeset in the same way as it is possible for the charges:

```
\ch{A_nB_m} \ch{H2SO4} \\
\chemsetup[chemformula]{subscript-style = math}
\ch{A_nB_m} \ch{H2SO4}
```

$\mathrm{A_nB_m}$ $\mathrm{H_2SO_4}$
$\mathrm{A}_n\mathrm{B}_m$ $\mathrm{H_2SO_4}$

The option adduct-space sets the space left and right to the adduct symbol ·.

```
\ch{Na3PO3*H2O} \\
\chemsetup[chemformula]{adduct-space=.2em}
\ch{Na3PO3*H2O}
```

$\mathrm{Na_3PO_3\cdot H_2O}$
$\mathrm{Na_3PO_3\,\cdot\,H_2O}$

Changing the length of the bonds:

```
\chemsetup[chemformula]{bond-length=4mm}%
single: \ch{CH3-CH3} \\
double: \ch{CH2=CH2} \\
triple: \ch{CH+CH}
```

single: $\mathrm{CH_3{-}CH_3}$
double: $\mathrm{CH_2{=}CH_2}$
triple: $\mathrm{CH{\equiv}CH}$

You can change the distance between bond and atom, too:

```
\ch{H-H + N+N + O=O} \\
\ch[bond-offset=1pt]{H-H + N+N + O=O}
```

$\mathrm{H{-}H + N{\equiv}N + O{=}O}$
$\mathrm{H{-}H + N{\equiv}N + O{=}O}$

6.7 Standalone Formulae

Introduced in version 4.0

CHEMFORMULA offers a command that *only accepts* the “compound” input type:

`\chcpd[<options>]{<compound>}`

7 Special Input Types

There are some “special type” input groups.

7.1 Single Token Groups

The first kind are groups which consist of only one token, namely of the following ones:

`\ch{ + }` +
Creates the plus sign between compounds with space around it:
`\ch{2 Na + Cl2}` $2\,\mathrm{Na} + \mathrm{Cl_2}$

`\ch{ v }` ↓
Sign for precipitate: `\ch{BaSO4 v}` $\mathrm{BaSO_4}\downarrow$

`\ch{ ^ }` ↑
Sign for escaping gas[7]: `\ch{H2 ^}` $\mathrm{H_2}\uparrow$

The space left and right of the plus sign can be set with this option:

`plus-space = <skip>` Default: `.3em plus .1em minus .1em`
A rubber length.

```
\ch{A + B}\\
\ch[plus-space=4pt]{A + B}
```

$\mathrm{A + B}$
$\mathrm{A\ +\ B}$

7.2 Option Input

Sometimes you might want to apply an option only to a part of a, say, reaction. Of course you have the possibility to use `\ch` several times.

```
\ch{H2O +}\textcolor{red}{\ch{H2SO4}}\ch{-> H3O+ + HSO4-} \\
\ch{H2O +}\ch[subscript-vshift=2pt]{H2SO4}\ch{-> H3O+ + HSO4-}
```

$\mathrm{H_2O + H_2SO_4 \longrightarrow H_3O^+ + HSO_4^-}$
$\mathrm{H_2O + H_2SO_4 \longrightarrow H_3O^+ + HSO_4^-}$

This, however, interrupts the input in your source and *may* mess with the spacing. That’s why there is an alternative:

`\ch{ @{<options>} }`
The options specified this way will be valid *only* until the next compound is set.

---

[7] Is this the correct English term? Please correct me if it isn’t.

```
\ch{H2O +}\textcolor{red}{\ch{H2SO4}}\ch{-> H3O+ + HSO4-} \\
\ch{H2O + @{format=\color{red}} H2SO4 -> H3O+ + HSO4-} \\
or of course:\\
\ch{H2O + \textcolor{red}{H2SO4} -> H3O+ + HSO4-}\\[1em]
\ch{H2O +}\ch[subscript-vshift=2pt]{H2SO4}\ch{-> H3O+ + HSO4-} \\
\ch{H2O + @{subscript-vshift=2pt} H2SO4 -> H3O+ + HSO4-}
```

$H_2O + H_2SO_4 \longrightarrow H_3O^+ + HSO_4^-$
$H_2O + H_2SO_4 \longrightarrow H_3O^+ + HSO_4^-$
or of course:
$H_2O + H_2SO_4 \longrightarrow H_3O^+ + HSO_4^-$

$H_2O + H_2SO_4 \longrightarrow H_3O^+ + HSO_4^-$
$H_2O + H_2SO_4 \longrightarrow H_3O^+ + HSO_4^-$

8 Escaped Input

In some cases it may be desirable to prevent CHEMFORMULA from parsing the input. This can be done in two ways.

8.1 Text

If you put something between `" "` or `' '` then the input will be treated as normal text, except that spaces are not allowed and have to be input with ~.

```
\ch{ "<escaped text>" }
```

```
\ch{ '<escaped text>' }
```

```
\ch{"\ox{2,Ca}" O} \\
\ch{"\ldots\," Na + "\ldots\," Cl2 -> "\ldots\," NaCl} \\
\ch{'A~->~B'}
```

$\overset{\text{II}}{\text{Ca}}\text{O}$
$\ldots\,\text{Na} + \ldots\,\text{Cl}_2 \longrightarrow \ldots\,\text{NaCl}$
A -> B

In many cases you won't need to escape the input. But when you get into trouble when using a command inside `\ch` try hiding it.

8.2 Math

If you especially want to input math you just enclose it with `$ $`. This output is different from the escaped text as it is followed by a space. The reasoning behind this is that I assume math will mostly be used to replace stoichiometric factors.

```
\ch{ $<escaped math>$ }
```

```
\ch{ \(<escaped math>\) }
```

```
escaped text: \ch{"$x$" H2O} \\
escaped math: \ch{$x$ H2O} \\
also escaped math: \ch{\(x\) H2O} \\
\ch{$2n$ Na + $n$ Cl2 -> $2n$ NaCl}
```

escaped text: $x\mathrm{H_2O}$
escaped math: $x\,\mathrm{H_2O}$
also escaped math: $x\,\mathrm{H_2O}$
$2n\,\mathrm{Na} + n\,\mathrm{Cl_2} \longrightarrow 2n\,\mathrm{NaCl}$

The space that is inserted after a math group can be edited:

`math-space = <skip>` Default: `.1667em plus .0333em minus .0117em`
A rubber length.

```
\ch{$2n$ Na + $n$ Cl2 -> $2n$ NaCl} \\
\chemsetup[chemformula]{math-space=.25em}
\ch{$2n$ Na + $n$ Cl2 -> $2n$ NaCl} \\
\ch{$A->B$}
```

$2n\,\mathrm{Na} + n\,\mathrm{Cl_2} \longrightarrow 2n\,\mathrm{NaCl}$
$2n\;\mathrm{Na} + n\;\mathrm{Cl_2} \longrightarrow 2n\;\mathrm{NaCl}$
$A->B$

9 Arrows

9.1 Arrow types

Arrows are input in the same intuitive way they are with mhchem. There are various different types:

`\ch{ -> }` $\longrightarrow$
standard right arrow

`\ch{ <- }` $\longleftarrow$
standard left arrow

`\ch{ -/> }` $\not\longrightarrow$
does not react (right)

`\ch{ </- }` </-
does not react (left)

`\ch{ <-> }` $\longleftrightarrow$
resonance arrow

`\ch{ <> }` $\rightleftarrows$
reaction in both directions

`\ch{ == }` $=$
stoichiometric equation

`\ch{ <=> }` $\rightleftharpoons$
equilibrium arrow

`\ch{ <=>> }` $\rightleftharpoons$
unbalanced equilibrium arrow to the right

`\ch{ <<=> }` $\leftharpoondown\!\!\!\!\!\relbar\!\!\rightharpoonup$

unbalanced equilibrium arrow to the left

`\ch{ <o> }` $\underset{o}{\longleftrightarrow}$

isolobal arrow

All these arrows are drawn with Ti*k*Z.

```
\ch{H2 + Cl2 -> 2 HCl} \\
\ch{H2O + CO3^2- <=> OH- + HCO3-} \\
\ch{A <- B} \\
\ch{\{[CH2=CH-CH2]- <-> [CH2-CH=CH2]- \}} \\
\ch{A <> B} \\
\ch{H+ + OH- <=>> H2O} \\
\ch{2 NO2 <<=> N2O4}
```

$$\mathrm{H_2 + Cl_2 \longrightarrow 2\,HCl}$$
$$\mathrm{H_2O + CO_3^{2-} \rightleftharpoons OH^- + HCO_3^-}$$
$$\mathrm{A \longleftarrow B}$$
$$\mathrm{\{[CH_2{=}CH{-}CH_2]^- \longleftrightarrow [CH_2{-}CH{=}CH_2]^-\}}$$
$$\mathrm{A \rightleftarrows B}$$
$$\mathrm{H^+ + OH^- \rightleftharpoons H_2O}$$
$$\mathrm{2\,NO_2 \rightleftharpoons N_2O_4}$$

9.2 Labels

The arrows take two optional arguments to label them.

`\ch{ ->[<above>][<below>] }`

```
\ch{A ->[a] B} \\
\ch{A ->[a][b] B} \\
\ch{A ->[\SI{100}{\celsius}] B}
```

$$\mathrm{A \xrightarrow{a} B}$$
$$\mathrm{A \xrightarrow[b]{a} B}$$
$$\mathrm{A \xrightarrow{100\,^{\circ}C} B}$$

The label text can be parsed seperately from the arrow. The recipe is easy: leave blanks.

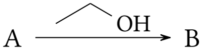
```
\ch{A ->[H2O] B} \\
\ch{A ->[ H2O ] B} \\
\ch{A ->[ "\ox{2,Ca}" F2 ] B} \\
\ch{A ->[$\Delta$,~ \[H+ \]] B}
```

$$\mathrm{A \xrightarrow{H2O} B}$$
$$\mathrm{A \xrightarrow{H_2O} B}$$
$$\mathrm{A \xrightarrow{\overset{II}{Ca}F_2} B}$$
$$\mathrm{A \xrightarrow{\Delta,\ [H^+]} B}$$

If you leave the blanks **CHEMFORMULA** treats the groups inside the square brackets as seperated input types. The arrow reads its arguments *afterwards*. As you can see the arrows “grow” with the length of the labels. What stays constant is the part that protrudes the labels. As you also can see in the last example square brackets inside the arrow arguments should be produced using `\[` and `\]`. They keep their usual meaning outside `\ch`. These commands are necessary since the usual grouping (i.e. hiding the brackets inside curly brackets) doesn’t work due to the way `\ch` reads its argument.

```
\ch{A ->[a] B} \\
\ch{A ->[ab] B} \\
\ch{A ->[abc] B} \\
\ch{A ->[abc~abc] B} \\
% needs the `chemfig' package:
\setatomsep{15pt}
\ch{A ->[ "\chemfig{-[:30]-[:-30]OH}" ] B} \\
\ch{A ->[[]] B} vs. \ch{A ->[\[\]] B}
```

$\mathrm{A} \xrightarrow{\text{a}} \mathrm{B}$
$\mathrm{A} \xrightarrow{\text{ab}} \mathrm{B}$
$\mathrm{A} \xrightarrow{\text{abc}} \mathrm{B}$
$\mathrm{A} \xrightarrow{\text{abc abc}} \mathrm{B}$



$\mathrm{A} \xrightarrow{[]} \mathrm{B}$ vs. $\mathrm{A} \xrightarrow{[]} \mathrm{B}$

9.3 Customization

These are the options which enable you to customize the arrows:

`arrow-offset = <dim>` Default: `.75em`

This is the length that an arrow protrudes a label on both sides. This means an empty arrow's length is two times `arrow-offset`.

`arrow-min-length = <dim>` Default: `0pt`

The minimal length an error must have unless two times `arrow-offset` plus the width of the label is larger.

`arrow-yshift = <dim>` Default: `0pt`

Shifts an arrow up (positive value) or down (negative value).

`arrow-ratio = <factor>` Default: `.6`

The ratio of the arrow lengths of the unbalanced equilibrium. `.4` would mean that the length of the shorter arrow is $0.4\times$ the length of the longer arrow.

`compound-sep = <dim>` Default: `.5em`

The space between compounds and the arrows.

`label-offset = <dim>` Default: `2pt`

The space between the labels and the arrows.

`label-style = <font command>` Default: `\footnotesize`

The relative font size of the labels.

The following code shows the effect of the different options on the <=>> arrow:

```
standard: \ch{A <=>>[x][y] B} \\
longer: \ch[arrow-offset=12pt]{A <=>>[x][y] B} \\
higher: \ch[arrow-yshift=2pt]{A <=>>[x][y] B} \\
more balanced: \ch[arrow-ratio=.8]{A <=>>[x][y] B} \\
labels further away: \ch[label-offset=4pt]{A <=>>[x][y] B} \\
larger distance to compounds: \ch[compound-sep=2ex]{A <=>>[x][y] B} \\
smaller labels: \ch[label-style=\tiny]{A <=>[x][y] B}
```

standard: A $\xrightleftharpoons[y]{x}$ B
longer: A $\xrightleftharpoons[y]{x}$ B
higher: A $\xrightleftharpoons[y]{x}$ B
more balanced: A $\xrightleftharpoons[y]{x}$ B
labels further away: A $\xrightleftharpoons[y]{x}$ B
larger distance to compounds: A $\xrightleftharpoons[y]{x}$ B
smaller labels: A $\xrightleftharpoons[y]{x}$ B

9.4 Modify Arrow Types

The arrows are defined with the command

`\DeclareChemArrow{<tokens>}{<tikz>}`

`{<tokens>}` is the sequence of tokens that is replaced with the actual arrow code. For example the basic arrow is defined via

```
\DeclareChemArrow{->}{\draw[-cf] (cf_arrow_start) -- (cf_arrow_end) ;}
```

In order to define arrows yourself you need to know the basics of TikZ.[8] There are some predefined coordinates you can and should use:

`(cf_arrow_start)` The beginning of the arrow.

`(cf_arrow_end)` The end of the arrow.

`(cf_arrow_mid)` The mid of the arrow.

`(cf_arrow_mid_start)` The beginning of the shorter arrow in types like <=>>.

`(cf_arrow_mid_end)` The end of the shorter arrow in types like <=>>.

`cf`, `left cf`, `right cf` CHEMFORMULA's own arrow heads.

```
\DeclareChemArrow{.>}{\draw[-cf,dotted,red] (cf_arrow_start) -- (cf_arrow_end);}
\DeclareChemArrow{n>}{\draw[-cf] (cf_arrow_start) .. controls ([yshift=3ex]cf_
 arrow_mid) .. (cf_arrow_end);}
\ch{A .> B} \ch{A .>[a][b] B} \ch{A n> B}
```

---

[8] Please see the pgfmanual for details.

A $\dashrightarrow$ B A $\overset{a}{\underset{b}{\dashrightarrow}}$ B A $\curvearrowright$ B

If you want to redefine an existing arrow there are two commands you can use:

```
\RenewChemArrow{<tokens>}{<tikz>}
```

```
\ShowChemArrow{<tokens>}
```

The second one gives the current definition, the first one redefines an existing arrow.

```
\texttt{\ShowChemArrow{->}} \\
\RenewChemArrow{->}{\draw[->,red] (cf_arrow_start) -- (cf_arrow_end) ;}
\texttt{\ShowChemArrow{->}} \\
\ch{A -> B}
```

```
\draw [-cf](cf_arrow_start)--(cf_arrow_end);
\draw [->,red] (cf_arrow_start) -- (cf_arrow_end) ;
```

A $\longrightarrow$ B

9.5 Standalone Arrows

Introduced in version 4.0

CHEMFORMULA offers a command that *only accepts* the “arrow” input type:

```
\charrow{<arrow>}[<above>][<below>]
```

10 Names

10.1 Syntax

CHEMFORMULA has a built-in syntax to write text under a compound. In a way it works very similar to the arrows.

```
\ch{ !(<name>)( <formula> ) }
```

If an exclamation mark is followed by a pair of parentheses CHEMFORMULA will parse it this way:

```
\ch{!(ethanol)( CH2CH2OH )}
```

$\underset{\text{ethanol}}{\mathrm{CH_2CH_2OH}}$

The same what’s true for the arrows arguments holds for these arguments: if you leave blanks the different parts will be treated according to their input type before the text is set below the formula.

```
\ch{!(water)(H2O)} \quad
\ch{!( "\textcolor{blue}{water}" )( H2O )} \quad
\ch{!( $2n-1$ )( H2O )} \quad
\ch{!( H2O )( H2O )} \quad
\ch{!(oxonium)( H3O+ )}
```

H2O	H_2O	H_2O	H_2O	H_3O^+
water	water	$2n-1$	H_2O	oxonium

If for some reason you want to insert an exclamation mark *without* it creating a name you only have to make sure it isn't followed by parentheses.

```
\ch{H2O~(!)} \\
\ch{A!{}()}
```

H2O (!)
A!()

10.2 Customization

CHEMFORMULA provides two options to customize the output of the names:

`name-format = <commands>` Default: `\scriptsize\centering`

The format of the name. This can be arbitrary input.

`name-width = <dim>|auto` Default: `auto`

The width of the box where the label is put into. `auto` will detect the width of the name and set the box to this width.

```
\ch{!(acid)( H2SO4 ) -> B} \\
\ch[name-format=\sffamily\small]{!(acid)( H2SO4 ) -> B} \\
\ch[name-format=\scriptsize N:~]{!(acid)( H2SO4 ) -> B} \\
\ch[name-width=3em,name-format=\scriptsize\raggedright]{!(acid)( H2SO4 ) -> B}
```

$\underset{\text{acid}}{H_2SO_4} \longrightarrow B$

$\underset{\text{acid}}{H_2SO_4} \longrightarrow B$

$\underset{\text{N: acid}}{H_2SO_4} \longrightarrow B$

$\underset{\text{acid}}{H_2SO_4} \longrightarrow B$

10.3 Standalone Names

Introduced in version 4.0

CHEMFORMULA offers a command that allows the usage of the "name" syntax in normal text. This is the command that a bang is replaced with in CHEMFORMULA's formulas, actually. Both arguments are mandatory.

`\chname(<under>)(<text>)`

11 Format and Font

In the standard setting CHEMFORMULA doesn't make any default changes to the font of the formula output. Let's take a look at a nonsense input which shows all features:

```
\newcommand*\sample{%
  \ch{H2C-C+C-CH=CH+ + CrO4^2-
      <=>[x][y]
    2.5 Cl^{-.} + 3_1/2 Na*OH_{(aq)} + !(name)( A^n ) "\LaTeXe"}
}
\sample
```

$$\mathrm{H_2C{-}C{\equiv}C{-}CH{=}CH^+ + CrO_4^{2-} \xrightleftharpoons[y]{x} 2.5\,Cl^{-\bullet} + 3\tfrac{1}{2}\,Na\cdot OH_{(aq)} + \underset{name}{A^n}\ \text{LaTeX}\,2_\varepsilon}$$

Now we're going to change different aspects of the font a look what happens:

```
\sffamily Hallo \sample \\
\ttfamily Hallo \sample \normalfont \\
\bfseries Hallo \sample \normalfont \\
\itshape Hallo \sample
```

$$\text{Hallo } \mathrm{H_2C{-}C{\equiv}C{-}CH{=}CH^+ + CrO_4^{2-} \xrightleftharpoons[y]{x} 2.5\,Cl^{-\bullet} + 3\tfrac{1}{2}\,Na\cdot OH_{(aq)} + \underset{name}{A^n}\ \text{LaTeX}\,2_\varepsilon}$$

$$\texttt{Hallo } \mathrm{H_2C{-}C{\equiv}C{-}CH{=}CH^+ + CrO_4^{2-} \xrightleftharpoons[y]{x} 2.5\,Cl^{-\bullet} + 3\tfrac{1}{2}\,Na\cdot OH_{(aq)} + \underset{name}{A^n}\ \text{LaTeX}\,2_\varepsilon}$$

$$\textbf{Hallo } \mathbf{H_2C{-}C{\equiv}C{-}CH{=}CH^+ + CrO_4^{2-} \xrightleftharpoons[y]{x} 2.5\,Cl^{-\bullet} + 3\tfrac{1}{2}\,Na\cdot OH_{(aq)} + \underset{name}{A^n}\ \text{LaTeX}\,2_\varepsilon}$$

$$\textit{Hallo } \mathit{H_2C{-}C{\equiv}C{-}CH{=}CH^+ + CrO_4^{2-} \xrightleftharpoons[y]{x} 2.5\,Cl^{-\bullet} + 3\tfrac{1}{2}\,Na\cdot OH_{(aq)} + \underset{name}{A^n}\ \text{LaTeX}\,2_\varepsilon}$$

As you can see most features adapt to the surrounding font.

If you want to change the default format you need to use this option:

`format = <anything>` (initially empty)

Adds arbitrary code before the output of `\ch`.

```
\definecolor{newblue}{rgb}{.1,.1,.5}
\chemsetup[chemformula]{format=\color{newblue}\sffamily}
\sffamily Hallo \sample \\
\ttfamily Hallo \sample \normalfont \\
\bfseries Hallo \sample \normalfont \\
\itshape Hallo \sample
```

$$\text{Hallo } \mathsf{H_2C{-}C{\equiv}C{-}CH{=}CH^+ + CrO_4^{2-} \xrightleftharpoons[y]{x} 2.5\,Cl^{-\bullet} + 3\tfrac{1}{2}\,Na\cdot OH_{(aq)} + \underset{name}{A^n}\ \text{LaTeX}\,2_\varepsilon}$$

$$\texttt{Hallo } \mathsf{H_2C{-}C{\equiv}C{-}CH{=}CH^+ + CrO_4^{2-} \xrightleftharpoons[y]{x} 2.5\,Cl^{-\bullet} + 3\tfrac{1}{2}\,Na\cdot OH_{(aq)} + \underset{name}{A^n}\ \text{LaTeX}\,2_\varepsilon}$$

$$\textbf{Hallo } \mathbf{\mathsf{H_2C{-}C{\equiv}C{-}CH{=}CH^+ + CrO_4^{2-} \xrightleftharpoons[y]{x} 2.5\,Cl^{-\bullet} + 3\tfrac{1}{2}\,Na\cdot OH_{(aq)} + \underset{name}{A^n}\ \text{LaTeX}\,2_\varepsilon}}$$

$$\textit{Hallo } \mathit{H_2C{-}C{\equiv}C{-}CH{=}CH^+ + CrO_4^{2-} \xrightleftharpoons[y]{x} 2.5\,Cl^{-\bullet} + 3\tfrac{1}{2}\,Na\cdot OH_{(aq)} + \underset{name}{A^n}\ \text{LaTeX}\,2_\varepsilon}$$

You can also specifically change the fontfamily, fontseries and fontshape of the output.

`font-family = <family>` (initially empty)

Changes the fontfamily of the output with `\fontfamily{<family>}\selectfont`.

`font-series = <series>` (initially empty)

Changes the fontseries of the output with `\fontseries{<series>}\selectfont`.

`font-shape = <shape>` (initially empty)

Changes the fontshape of the output with `\fontshape{<shape>}\selectfont`.

```
\chemsetup[chemformula]{font-series=bx}
Hallo \sample \\
\sffamily Hallo \sample \normalfont \\
\chemsetup[chemformula]{font-family=lmr,font-series=m} Hallo \sample \normalfont \\
\itshape Hallo \sample
```

Hallo $\mathbf{H_2C{-}C{\equiv}C{-}CH{=}CH^+ + CrO_4^{2-} \xrightleftharpoons[y]{x} 2.5\,Cl^{-\bullet} + 3\tfrac{1}{2}\,Na{\cdot}OH_{(aq)} + \underset{name}{A^n}}\ \text{\LaTeX}\,\mathbf{2}_{\varepsilon}$

Hallo $\mathsf{\mathbf{H_2C{-}C{\equiv}C{-}CH{=}CH^+ + CrO_4^{2-} \xrightleftharpoons[y]{x} 2.5\,Cl^{-\bullet} + 3\tfrac{1}{2}\,Na{\cdot}OH_{(aq)} + \underset{name}{A^n}}}\ \text{\LaTeX}\,\mathbf{2}_{\varepsilon}$

Hallo $\mathrm{H_2C{-}C{\equiv}C{-}CH{=}CH^+ + CrO_4^{2-} \xrightleftharpoons[y]{x} 2.5\,Cl^{-\bullet} + 3\tfrac{1}{2}\,Na \cdot OH_{(aq)} + \underset{name}{A^n}}\ \text{\LaTeX}\,2_{\varepsilon}$

Hallo $H_2C{-}C{\equiv}C{-}CH{=}CH^+ + CrO_4^{2-} \xrightleftharpoons[y]{x} 2.5\,Cl^{-\bullet} + 3\tfrac{1}{2}\,Na \cdot OH_{(aq)} + \underset{name}{A^n}\ \text{\LaTeX}\,2_{\varepsilon}$

If you're using XeLaTeX or LuaLaTeX and have loaded fontspec[9] you have the possibilty to set the font with it:

`font-spec = {<font>}` (initially empty)

or with options

`font-spec = {[<options>]<font>}`

```
\chemsetup[chemformula]{font-spec={Linux Biolinum O}} \sample \\
\chemsetup[chemformula]{font-spec={Augie}} \sample \\
\chemsetup[chemformula]{font-spec={Latin Modern Sans}} \sample \\
\bfseries \sample \normalfont
```

$\mathsf{H_2C{-}C{\equiv}C{-}CH{=}CH^+ + CrO_4^{2-} \xrightleftharpoons[y]{x} 2.5\,Cl^{-\bullet} + 3\tfrac{1}{2}\,Na{\cdot}OH_{(aq)} + \underset{name}{A^n}}\ \text{\LaTeX}\,2_{\varepsilon}$

$H_2C{-}C{\equiv}C{-}CH{=}CH^+ + CrO_4^{2-} \xrightleftharpoons[y]{x} 2.5\,Cl^{-\bullet} + 3\tfrac{1}{2}\,Na{\cdot}OH_{(aq)} + \underset{name}{A^n}\ \text{\LaTeX}\,2_{\varepsilon}$

$\mathsf{H_2C{-}C{\equiv}C{-}CH{=}CH^+ + CrO_4^{2-} \xrightleftharpoons[y]{x} 2.5\,Cl^{-\bullet} + 3\tfrac{1}{2}\,Na \cdot OH_{(aq)} + \underset{name}{A^n}}\ \text{\LaTeX}\,2_{\varepsilon}$

$\mathsf{\mathbf{H_2C{-}C{\equiv}C{-}CH{=}CH^+ + CrO_4^{2-} \xrightleftharpoons[y]{x} 2.5\,Cl^{-\bullet} + 3\tfrac{1}{2}\,Na \cdot OH_{(aq)} + \underset{name}{A^n}}}\ \text{\LaTeX}\,2_{\varepsilon}$

12 Usage In Math Equations

The `\ch` command can be used inside math equations. It recognizes `\\` and `&` and passes them on. However, you can't use the optional arguments of `\\` inside `\ch`.

---

[9] on CTAN: fontspec

```
\begin{align}
 \ch{
   H2O & ->[a] H2SO4 \\
   Cl2 & ->[x][y] CH4
 }
\end{align}
\begin{align*}
\ch{
  RNO2      &<=>[ + e- ] RNO2^{-.} \\
  RNO2^{-.} &<=>[ + e- ] RNO2^2-
}
\end{align*}
```

$$H_2O \xrightarrow{a} H_2SO_4 \tag{1}$$

$$Cl_2 \xrightarrow[y]{x} CH_4 \tag{2}$$

$$\begin{aligned} RNO_2 &\xrightleftharpoons{+\,e^-} RNO_2^{-\bullet} \\ RNO_2^{-\bullet} &\xrightleftharpoons{+\,e^-} RNO_2^{2-} \end{aligned}$$

13 Further Examples

This section presents some examples of a possible usage.

```
\begin{reaction}[Synthese von Alkanen]
 !(Synthesegas)( $n$ CO + $(2n+1)$ H2 )
 ->[\SI{200}{\celsius}][\[CoNi\]]
 C_{$n$}H_{$2n+2$} + $n$ H2O
\end{reaction}
```

$$\underset{\text{Synthesegas}}{n\,CO + (2n+1)\,H_2} \xrightarrow[\text{[CoNi]}]{200\,^{\circ}C} C_nH_{2n+2} + n\,H_2O \tag*{\{1\}}$$

```
\begin{reactions*}
 "a)" && CH4    + Cl2 &-> CH3Cl  + HCl && "{\small Chlormethan/Methylchlorid}"
 \\
 "b)" && CH3Cl  + Cl2 &-> CH2Cl2 + HCl && "{\small Dichlormethan/Methylenchlorid
 }" \\
 "c)" && CH2Cl2 + Cl2 &-> CHCl3  + HCl && "{\small Trichlormethan/Chloroform}"
 \\
 "d)" && CHCl3  + Cl2 &-> CCl4   + HCl && "{\small Tetrachlormethan/
 Tetrachlorkohlenstoff}"
\end{reactions*}
```

$$\begin{aligned}
&\text{a)} && CH_4 + Cl_2 \longrightarrow CH_3Cl + HCl && \text{Chlormethan/Methylchlorid} \\
&\text{b)} && CH_3Cl + Cl_2 \longrightarrow CH_2Cl_2 + HCl && \text{Dichlormethan/Methylenchlorid} \\
&\text{c)} && CH_2Cl_2 + Cl_2 \longrightarrow CHCl_3 + HCl && \text{Trichlormethan/Chloroform} \\
&\text{d)} && CHCl_3 + Cl_2 \longrightarrow CCl_4 + HCl && \text{Tetrachlormethan/Tetrachlorkohlenstoff}
\end{aligned}$$

```
\chemsetup[ox]{parse=false}
\ch{"\ox{\delm,C}" -{} "\ox{\delp,M}" \qquad ( <-> "\ox{\delp,C}" -{} "\ox{\delm,Br}" )} \\
\ch[adduct-space=0pt]{X. + .Y <=> X-Y + Bindungsenergie} \\
\ch[name-format=\normalsize]{
  !(\State{H}{f}\qquad)() !(\textcolor{red}{??})( CH4\gas{} ) +
  !(\num{0})( 2 O2\gas{} )
  ->
  !(\num{-94.3})( CO2\gas{} ) +
  !(\num{-57.9})( H2O\lqd{} ) +
  !(\num{-192.1})( "\State{H}" )
}
```

$$\overset{\delta-}{\mathrm{C}}-\overset{\delta+}{\mathrm{M}} \qquad (\longleftrightarrow \overset{\delta+}{\mathrm{C}}-\overset{\delta-}{\mathrm{Br}})$$

$$\mathrm{X}\cdot + \cdot\mathrm{Y} \rightleftharpoons \mathrm{X{-}Y} + \text{Bindungsenergie}$$

$$\begin{array}{llllll} & \mathrm{CH_4\,(g)} + & \mathrm{2\,O_2\,(g)} \longrightarrow & \mathrm{CO_2\,(g)} + & \mathrm{H_2O\,(l)} + & \Delta H^\ominus \\ \Delta_\mathrm{f}H^\ominus & ?? & 0 & -94.3 & -57.9 & -192.1 \end{array}$$

```
\newcommand\cstack[1]{%
  \clap{%
    \begin{tabular}{c}
      #1
    \end{tabular}
  }%
}
\begin{reactions*}
 CH3MgBr + "\ox*{1,Cu}" X &-> "\glqq" CH3 "\ox*{1,Cu}\grqq" + MgBrX "\qquad X ~$=$~Br,I,CN" \\
 2 MeLi + CuI             &-> !(\cstack{Dimethylcuprat\\(Gilmann-Cuprat)})( Me2CuLi ) + Li
\end{reactions*}
```

$$\mathrm{CH_3MgBr} + \mathrm{Cu^{I}X} \longrightarrow „\mathrm{CH_3Cu^{I}}“ + \mathrm{MgBrX} \qquad \mathrm{X} = \mathrm{Br,I,CN}$$

$$2\,\mathrm{MeLi} + \mathrm{CuI} \longrightarrow \underset{\substack{\text{Dimethylcuprat}\\\text{(Gilmann-Cuprat)}}}{\mathrm{Me_2CuLi}} + \mathrm{Li}$$

```
% needs `chemfig'
\begin{reactions*}
 H3C-CH3 + Cl2                        &->[$\Delta$][$h\nu$] H3CCH2Cl + HCl
     & &"\Enthalpy{-27.1}" \\
 H3C-CH3 + "\Lewis{0.,Cl}"            &-> H3CCH2 "\Lewis{0.,\vphantom{H}}" + HCl & &"\Enthalpy{-5.0}" \\
 H3C-CH2 "\Lewis{0.,\vphantom{H}}" + Cl2 &-> H3CCH2Cl + "\Lewis{0.,Cl}"
     & &"\Enthalpy{-23.0}"
\end{reactions*}
```

$$\begin{aligned}
H_3C{-}CH_3 + Cl_2 &\xrightarrow[h\nu]{\Delta} H_3CCH_2Cl + HCl & \Delta H^\ominus &= -27.1\,\mathrm{kJ\,mol^{-1}}\\
H_3C{-}CH_3 + Cl^{\bullet} &\longrightarrow H_3CCH_2{}^{\bullet} + HCl & \Delta H^\ominus &= -5.0\,\mathrm{kJ\,mol^{-1}}\\
H_3C{-}CH_2{}^{\bullet} + Cl_2 &\longrightarrow H_3CCH_2Cl + Cl^{\bullet} & \Delta H^\ominus &= -23.0\,\mathrm{kJ\,mol^{-1}}
\end{aligned}$$

The following example shows how the cancelling of compounds could be done.[10]

```
% needs `cancel'
\begin{align*}
 \ch{\cancel{HCOOH\aq} + H2O\lqd{}  &<=> H3O^+\aq{} + \cancel{HCOO^-\aq}} \\
 \ch{\cancel{HCOO^-\aq} + H2O\lqd{} &<=> \cancel{HCOOH\aq} + OH^-\aq}\\[-1ex]
 \cline{1-2}
 \ch{H2O\lqd{} + H2O\lqd{} &<=> H3O^+\aq{} + OH^-\aq}
\end{align*}
```

$$\begin{array}{rcl}
\cancel{HCOOH\,(aq)} + H_2O\,(l) & \rightleftharpoons & H_3O^+\,(aq) + \cancel{HCOO^-\,(aq)}\\
\cancel{HCOO^-\,(aq)} + H_2O\,(l) & \rightleftharpoons & \cancel{HCOOH\,(aq)} + OH^-\,(aq)\\
\hline
H_2O\,(l) + H_2O\,(l) & \rightleftharpoons & H_3O^+\,(aq) + OH^-\,(aq)
\end{array}$$

References

[Coh+08] E. Richard Cohan, Tomislav Cvitaš, Jeremy G. Frey, Bertil Holmström, Kozo Kuchitsu, Roberto Marquardt, Ian Mills, Franco Pavese, Martin Quack, Jürgen Stohner, Herbert L. Strauss, Michio Takami, and Anders J Thor. *"Quantities, Symbols and Units in Physical Chemistry", IUPAC Green Book.* 3rd Edition. 2nd Printing. IUPAC & RSC Publishing, Cambridge, 2008.

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[10] Inspired by a question on TeX.SE: `http://tex.stackexchange.com/q/30118/5049`

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Section titles are indicated **bold**, packages sans serif, commands \brown, options yellow and modules (only CHEMMACROS) blue.