

# the chemmacros bundle

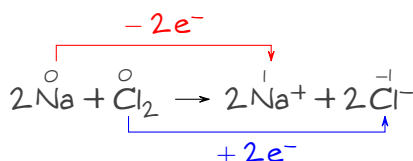
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packages `chemmacros`, `chemformula` and `ghsystem`

Clemens NIEDERBERGER

<https://bitbucket.org/cgnieder/chemmacros/>  
[contact@mychemistry.eu](mailto:contact@mychemistry.eu)

English documentation



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# Part I.

## Preliminaries

### 1. Licence, Requirements and README

The `CHEMMACROS` bundle underlies the L<sup>A</sup>T<sub>E</sub>X project public license (lppl) version 1.3 or later (<http://www.latex-project.org/lppl.txt>) and has the status “maintained.”

The `CHEMMACROS` bundle needs the bundles `l3kernel`<sup>1</sup> and `l3packages`.<sup>2</sup> It also needs the packages `siunitx`,<sup>3</sup> `mathtools`,<sup>4</sup> `bm`,<sup>5</sup> `nicefrac`<sup>6</sup> and `environ`<sup>7</sup> as well as `tikz`<sup>8</sup> and the T<sub>i</sub>kZ libraries `calc` and `arrows`.

Package option `bpchem` (section 4) needs the package `bpchem`,<sup>9</sup> package option `xspace` needs the package `xspace`<sup>10</sup> and package option `method = mhchem` needs the package `mhchem`.<sup>11</sup>

With v3.0 the `CHEMMACROS` package has been bundled with the new packages `CHEMFORMULA` and `GHSYSTEM`. `CHEMFORMULA` provides an alternative to `mhchem`. This leads to some internal changes in `CHEMMACROS`. On the same time the documentation has been redesigned.

You might remember that `CHEMMACROS`’ options all belong to different modules, see section 5 for further information. These are typeset in the left margin when the option is first mentioned. In section V all options and the module they belong to are listed. Throughout the document options are typeset green and modules red.

The package `GHSYSTEM` needs the packages `CHEMMACROS`, `tabu`,<sup>12</sup> `longtable`,<sup>13</sup> `ifpdf`<sup>14</sup> and `graphicx`.<sup>15</sup> `GHSYSTEM` has no own package options but passes all options on to `CHEMMACROS`.

There are some deprecated commands and options which are not explained in the manual any more but still exist to ensure backwards compatibility. These commands issue a warning. They may be dropped some time in the future.

### 2. Motivation and Background

`CHEMMACROS` started some years ago as a growing list of custom macros that I frequently used. I cannot completely recall when and why I decided to release them as a package. Well – here we go and you might find it useful, too, I hope.

<sup>1</sup> CTAN: `l3kernel`   <sup>2</sup> CTAN: `l3packages`   <sup>3</sup> CTAN: `siunitx`   <sup>4</sup> CTAN: `mathtools`   <sup>5</sup> CTAN: `bm`   <sup>6</sup> CTAN: `nicefrac`  
<sup>7</sup> CTAN: `environ`   <sup>8</sup> CTAN: `pgf`   <sup>9</sup> CTAN: `bpchem`   <sup>10</sup> CTAN: `xspace`   <sup>11</sup> CTAN: `mhchem`   <sup>12</sup> CTAN: `tabu`   <sup>13</sup> CTAN: `longtable`   <sup>14</sup> CTAN: `ifpdf`   <sup>15</sup> CTAN: `graphicx`

## 2. Motivation and Background

Both the macros and their functionality have changed over time and quite a lot have been added. Many things have been unified and what's probably most important: many possibilities to customize have been added, too.

Probably every chemist using  $\text{\LaTeX}$  2 $\epsilon$  is aware of the great mhchem 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 possibilities to customize the output that mhchem does not. Since CHEMFORMULA is meant as an *alternative* to mhchem CHEMMACROS offers a package option allowing you to choose which one of the two is used. The default however is CHEMMACROS own way: CHEMFORMULA.

As a chemist you are probably aware of the fact that the UNITED NATIONS have developed the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) as a global replacement for the various different systems in different countries. While it has not been implemented by all countries yet [Eur12], it is only a matter of time.

The package GHSYSTEM now enables you to typeset all the hazard and precautionary statements and pictograms in a very easy way. The statements are taken from EU regulation 1272/2008 [Theo8].

There are four points I hope I have achieved with this bundle:

- intuitive usage as far as the syntax of the commands is concerned
- the commands shall not only make typesetting easier and faster but also the document source more readable with respect to semantics (`\ortho`-dichlorobenzene is easier to read and understand than `\textsl{o}`-dichlorobenzene)
- as much customizability as I could think of so every user can adapt the commands to his or her own wishes
- default settings compliant with the recommendations of the International Union of Pure and Applied Chemistry (IUPAC).

Especially the last point needed some pushing from users to get things right in many places. If you find anything not compliant with IUPAC recommendations<sup>16</sup> I would welcome an email very much!

In a package this large with older parts and rather new parts (which have to be considered being in beta state) it is unavoidable that there are flaws and bugs. I am very keen on correcting and improving this package, so please: if you find anything that bothers you and may it be just so small please send me a short email and I'll see what I can do. I would especially like feedback on CHEMFORMULA (see part III) and GHSYSTEM (see part IV) but also welcome feedback on every other part of this bundle.

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<sup>16</sup> This does not concern the `\ox` command. The IUPAC version is `\ox*`.

### 3. Installation, Loading the Bundle

The bundle comes with three style files,<sup>17</sup> a directory called `language/` containing the language-definition files for GHS (ending `def`), and a directory `pictures/` containing `eps`, `pdf`, `jpg` and `png` files (the GHS pictograms). If you install the bundle manually *please make sure to place the directories `language/` and `pictures/` in the same directory as the style files.*

Loading **CHEMMACROS** with

```
1 \usepackage{chemmacros} % 'chemmacros', 'chemformula' and 'ghsystem' are
   loaded
```

will also load **CHEMFORMULA** and **GHSYSTEM**. However, you can prevent **CHEMMACROS** from loading **GHSYSTEM**:

```
1 \usepackage[ghsystem=false]{chemmacros} % 'chemmacros' and 'chemformula' are
   loaded
```

Loading **CHEMFORMULA** or **GHSYSTEM** explicitly is possible and will also load **CHEMMACROS** if it hasn't been loaded yet, and will therefore implicitly load the other package, too.

```
1 \usepackage{chemformula}
2 or
3 \usepackage{ghsystem}
```

However, it is recommended to simply use `\usepackage{chemmacros}` and setup the required options with `\chemsetup` (also see section 5).

### 4. Package Options

**CHEMMACROS** has several package options. They all are used as key/value pairs like

```
1 \usepackage[option1 = <value1>, option2 = <value2>]{chemmacros}
```

Some also can be used without value (`\usepackage[option1]{chemmacros}`), which means that the underlined value is used.

Both **CHEMFORMULA** and **GHSYSTEM** don't have package options of their own. If you load them explicitly any given option will silently fail. Options can then only be set using the setup command.

**option** ► **bpchem** = true|false → This option loads the package `bpchem` and adjusts the layout of the `\NMR` command to the `bpchem` commands `\HNMR` and `\CNMR`. (default = false)

**option** ► **circled** = formal|all|none → **CHEMMACROS** uses two different kinds of charges which indicate the

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<sup>17</sup> Those ending `sty`.

## 5. Setup

usage of real (+/−) and formal ( $\oplus/\ominus$ ) charges. The option `formal` distinguishes between them, option `none` displays them all without circle, option `all` circles all (default = `formal`)

**option** ▶ `circltype` = `chem|math` → This option switches between two kinds of circled charge symbols: `\fplus`  $\oplus$  and `\oplus`  $\oplus$ . (default = `chem`)

**option** ▶ `cmversion` = `1|2|bundle` → This option restores the old definitions of some commands, so documents set with `v1.*` will still compile correctly. (default = `bundle`). Actually `2` and `bundle` are only aliases. *This option can only be chosen in the preamble.*

**option** ▶ `ghsystem` = `true|false` → Disable the use of the `GHSYSTEM` package. Setting `ghs` = `false` will prevent `CHEMMACROS` from loading `GHSYSTEM`. (default = `true`)

**option** ▶ `greek` = `math|textgreek|upgreek` → This Options determines how the letters `\Chemalpha` and friends are typeset. See page 10 for more information. *This option can only be chosen in the preamble.* (default = `upgreek`)

**option** ▶ `iupac` = `auto|restricted|strict` → Take care of how IUPAC naming commands are defined, see page 12 (default = `auto`)

**option** ▶ `language` = `american|british|english|french|german|italian|ngerman` → Load language specific options. `english`, `american` and `british` are aliases, as are `german` and `ngerman`. *This option can only be chosen in the preamble.* (default = `english`).

**option** ▶ `method` = `chemformula|mhchem` → You can choose the method which `CHEMMACROS` will use for the reaction environments (see section 18) and the typesetting of the particles (see section 8). (default = `chemformula`). *This option can only be chosen in the preamble.*

**option** ▶ `Nu` = `chemmacros|mathspec` → The package `mathspec`<sup>18</sup> also defines a macro `\Nu`. This option chooses which definition holds, see page 9. (default = `chemmacros`). *This option can only be chosen in the preamble.*

**option** ▶ `strict` = `true|false` → Setting `strict` = `true` will turn all warning messages into errors messages. (default = `false`)

**option** ▶ `synchronize` = `true|false` → The setting `true` will tell `CHEMMACROS` the adapt the font settings of `CHEMFORMULA` if that method has been chosen (default = `false`). In order to demonstrate this feature this document is set with `synchronize` = `true` and the `CHEMFORMULA` setting `\chemsetup[chemformula]{font-spec={[[Color=darkgray]Latin Modern Sans}}`.

**option** ▶ `xspace` = `true|false` → With this option most commands are defined with a `\xspace`. (default = `true`)

## 5. Setup

Various of `CHEMMACROS`’, `CHEMFORMULA`’s and `GHSYSTEM`’s commands have key/value pairs with which they can be customized. Most times they can be used as (optional) argument of the commands themselves. They also can most times be used with the `\chemsetup` command.

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<sup>18</sup> CTAN: `mathspec`

## 6. Language Settings

► `\chemsetup[<module>]{<key> = <value>}` or

► `\chemsetup{<module>/<key> = <value>}`

The keys each belong to a module, which defines for which commands they are intended for. If a key is presented, you'll see the module to which it belongs in the left margin. You have two ways to use keys with the `\chemsetup`, as you can see above.

**option** The package options can also be seen as keys belonging to the module **option**. This means they can also be used with the `\chemsetup` command (except for the option `version = 1/2/3`).

```
1 \chemsetup[option]{circled=none}\mch\ \pch\ \fmch\ \fpch\ \el\ \prt \\  
2 \chemsetup[option]{circled=formal}\mch\ \pch\ \fmch\ \fpch\ \el\ \prt \\  
3 \chemsetup[option]{circletype=math}\mch\ \pch\ \fmch\ \fpch\ \el\ \prt \\  
4 \chemsetup{option/circletype=chem,option/circled=all}\mch\ \pch\ \fmch\ \fpch\ \  
5 \el\ \prt \\  
6 \chemsetup{option/circletype=math}\mch\ \pch\ \fmch\ \fpch\ \el\ \prt \\  
  
- + - + e- p+  
- + ⊖ ⊕ e- p+  
- + ⊖ ⊕ e- p+  
⊖ ⊕ ⊖ ⊕ e⊖ p⊕  
⊖ ⊕ ⊖ ⊕ e⊖ p⊕
```

Keys *not* belonging to a module *cannot* be used with `\chemsetup`!

All options of **CHEMFORMULA** belong to the module **chemformula** and all of **GHSYSTEM**'s options belong to the module **ghs**.

## 6. Language Settings

### 6.1. Supported Languages

By choosing the option

```
1 \chemsetup[option]{language=<language>}
```

you can set one of these languages: american, british, codeenglish, french, german, italian and ngerman. The languages american, british and english are aliases, as are german and ngerman.

These translate

- The header of the list of reactions.
- The beginning of the entries in the list of reactions.
- The H- and P-statements of the GHS.

Please note, that the GHS statements are not provided in all languages, see also section 36.

## 6.2. Specialties

### 6.2.1. German

If you choose `german/ngerman` the phase commands `\sld` and `\lqd` and the command `\pKa` are translated.

### 6.2.2. Italian

Choosing the language `italian` defines two additional IUPAC commands:

► `\ter` → *ter*

► `\sin` → *sin*

## 7. News

### 7.1. Version 3.3

- With v3.3 there is the environment `\begin{experimental}` `\end{experimental}`, see section 16. It can be used together with some new options and commands for the consistent typesetting of experimental data.
- The environment `\begin{reaction}` `\end{reaction}` and its kin can now cope with `\label`, `\ref` and `\intertext`, see section 18.
- The package options `german` and `ngerman` are deprecated, the replacement is `language`, see page 6 and section 6 from page 7.
- The package option `upgreek` got renamed into `greek`.
- Some additional `\Chem<greekletter>`-commands are provided, see section 8.

### 7.2. Version 3.3a

- The IUPAC commands `\hapto` and `\bridge` are new.
- The H and P statements now are available in Italian.

### 7.3. Version 3.3d

- pdf versions of the GHS pictograms.
- New default values for bond length and bond offset, see page 49.
- New option `bond-style`, see page 49.
- new option `cip-kern`, see page 14.



## 7.4. Version 3.4

- **CHEMMACROS** got an Italian manual, many thanks to Jonas Rivetti who volunteered to not only translate the H & P statements but also this documentation!
- the command `\bond` which allows to use other bonds than single, double and triple, see section 25.5. I wanted to add this for a long time!
- a few changes to the looks of the radical point and new options to customize it, see section 25.6.

## Part II.

# chemmacros

## 8. Particles, Ions and Symbols

### 8.1. Predefined

**CHEMMACROS** defines some simple macros for displaying often needed particles and symbols. Please note, that they're displayed differently depending on the package options used, see section 4. These commands can be used in text as well as in math mode.

- ▶ `\Hp1` →  $\text{H}^+$  (proton)
- ▶ `\Hyd` →  $\text{OH}^-$  (hydroxide)
- ▶ `\HtO` →  $\text{H}_3\text{O}^+$  (oxonium ion) (H three O)
- ▶ `\water` →  $\text{H}_2\text{O}$
- ▶ `\el` →  $\text{e}^-$  (electron)
- ▶ `\prt` →  $\text{p}^+$  (proton)
- ▶ `\ntr` →  $\text{n}^0$  (neutron)
- ▶ `\Nu` →  $\text{Nu}^-$  (nucleophile). The package **mathspec** also defines a macro `\Nu`. If you chose package option `Nu = mathspec` **CHEMMACROS** defines `\Nuc` instead.
- ▶ `\El` →  $\text{E}^+$  (electrophile)
- ▶ `\ba` →  $\text{ba}^-$  (base)
- ▶ `\fplus` →  $\oplus$
- ▶ `\fminus` →  $\ominus$
- ▶ `\transitionstatesymbol` →  $\ddagger$

- ▶ `\standardstate`  $\rightarrow \ominus$ . This symbol is only provided by `CHEMMACROS`, if the package `chemstyle`<sup>19</sup> is not loaded; the idea is borrowed from there.<sup>20</sup>
- ▶ `\Chemalpha`  $\rightarrow \alpha$
- ▶ `\Chembeta`  $\rightarrow \beta$
- ▶ `\Chemgamma`  $\rightarrow \gamma$
- ▶ `\Chemdelta`  $\rightarrow \delta$
- ▶ `\Chemepsilon`  $\rightarrow \varepsilon$
- ▶ `\Chemeta`  $\rightarrow \eta$
- ▶ `\Chemkappa`  $\rightarrow \kappa$
- ▶ `\Chemmu`  $\rightarrow \mu$
- ▶ `\Chemnu`  $\rightarrow \nu$
- ▶ `\Chemrho`  $\rightarrow \rho$
- ▶ `\Chempi`  $\rightarrow \pi$
- ▶ `\Chemsigma`  $\rightarrow \sigma$
- ▶ `\Chemomega`  $\rightarrow \omega$
- ▶ `\ChemDelta`  $\rightarrow \Delta$

The command `\Rad` has been dropped!

The two particles `\Nu` and `\ba` can be modified. To do that you use the option

`particle` ▶ `elpair` = `false|dots|dash`.

It only has any effect, if the package `chemfig`<sup>21</sup> is loaded, since it uses it's command `\Lewis`.

```

1 % needs package 'chemfig'
2 \ba[elpair] \Nu[elpair=dash]
3
4 \chemsetup[particle]{elpair}
5 \ba \Nu

```

$\text{ba}^{\cdot-} \text{Nu}^{\cdot-}$   
 $\text{ba}^{\cdot-} \text{Nu}^{\cdot-}$

The greek letters aren't newly defined symbols but are defined differently depending on the packages you've loaded. The default definition is the corresponding math letter. If you have loaded the `textgreek`<sup>22</sup> package the letters are taken from there, and if you have loaded the package `upgreek`<sup>23</sup> the macros of that package are used. This documentation uses `upgreek` for instance. If you load both `upgreek` and `textgreek` the letters from `upgreek` are used.

Table 1: The greek letters

	math	upgreek	textgreek
<code>\Chemalpha</code>	$\alpha$	$\alpha$	$\alpha$
<code>\Chembeta</code>	$\beta$	$\beta$	$\beta$
<code>\ChemDelta</code>	$\Delta$	$\Delta$	$\Delta$

If you don't want `CHEMMACROS` to use a package automatically but want to decide for yourself, there is the option `greek`. Table 1 shows the different styles for some of the letters.

The reason why `CHEMMACROS` defines these macros in the first place is IUPAC compliance. IUPAC recommends to use upright greek letters in nomenclature.

Greek letters are used in systematic organic, inorganic, macromolecular and biochemical nomenclature. These should be roman (upright), since they are not symbols for physical quantities. *IUPAC Green Book* [Coh+08, p. 9]

`CHEMMACROS` uses these commands now to defined nomenclature commands, see page 13.

## 8.2. Own Particles

Surely sometimes it can be handy to have other particle macros defined such as `\positron` or `\photon`. This can easily be done with this command:

► `\DeclareChemParticle{<cmd>}{<definition>}`

► `\RenewChemParticle{<cmd>}{<definition>}`

Depending on the `method` you chose as option the `<definition>` will either be a formula defined with `mhchem` or with `CHEMFORMULA`. The particle defined this way behaves like the predefined ones with one exception: if you chose `method = mhchem` the particle *will not* obey the option `circled`. If you want formal charges with this method you need to use `CHEMMACROS`' commands (see section 12) explicitly. If you chose `method = chemformula` the particle *will* obey the `circled` option.

```

1 % uses the 'upgreek' package
2 \DeclareChemParticle{\positron}{$\upbeta$+}
3 \DeclareChemParticle{\photon}{$\upgamma$}
4 \RenewChemParticle{\el}{$\upbeta$-}
5 \positron\ \photon\ \el

```

$$\beta^+ \gamma \beta^-$$

`\DeclareChemParticle` only defines a particle if `<cmd>` is not already used by any other command. If it is already used `CHEMMACROS` will either give a warning or an error, depending on the option `strict`. `\RenewChemParticle` *only* defines a particle if `<cmd>` is already used and issues a warning/error otherwise.

<sup>19</sup> CTAN: `chemstyle` <sup>20</sup> many thanks to the package author Joseph Wright. <sup>21</sup> CTAN: `chemfig` <sup>22</sup> CTAN: `textgreek`

<sup>23</sup> CTAN: `upgreek`

## 9. Nomenclature, Stereo Descriptors, Latin Phrases

### 9.1. IUPAC Names

Similar to the bpchem package CHEMMACROS provides a command<sup>24</sup> to typeset IUPAC names. Why is that useful? IUPAC names can get very long. So long indeed that they span over more than two lines, especially in two-column documents. This means they must be allowed to be broken more than one time. This is what the following command does.

- `\iupac{<IUPAC name>}` Inside this command use `\|` and `\-` to indicate a breaking point or a breaking dash. Use `\^` as a shortcut for `\textsuperscript`.<sup>25</sup>

```
1 \begin{minipage}{.4\linewidth}
2 \iupac{Tetra\|cyclo[2.2.2.1\^{1,4}]\-un\|decane-2\|-dodecyl\|-5\-(hepta\|decyl\|
   iso\|dodecyl\|thio\|ester)}
3 \end{minipage}

Tetracyclo[2.2.2.11,4]-undecane-2-do-
decyl-5-(heptadecylisododecylthioes-
ter)
```

The `\iupac` command is more of a semantic command. Most times you can achieve (nearly) the same thing by using `\-` instead of `\|`, `-` instead of `\-` and `\textsuperscript` instead of `\^`.

There are some subtleties: `\-` inserts a small space before the hyphen and removes a small space after it. The command `\|` not only prevents ligatures but also inserts a small space.

```
1 \huge\iupac{2,4-Di\|chlor\|pentan} \|
2 2,4-Dichlorpentan
```

2,4-Dichlorpentan  
2,4-Dichlorpentan

The spaces inserted by these commands can be customized.

`iupac` ► `hyphen-pre-space` = <dim> → Default = .01em

`iupac` ► `hyphen-post-space` = <dim> → Default = -.03em

`iupac` ► `break-space` = <dim> → Default = .01em

The command `\iupac` serves another purpose, too, however. Regardless of the setting of the `iupac` option all the commands presented in this section are always defined *inside* `\iupac`. Quite a number of the naming commands have very general names: `\meta`, `\D`, `\E`, `\L`, `\R`, `\S`, `\trans` and so forth. This means they either are predefined already (`\L` `\L`) or are easily defined by another package or class (the `cool`<sup>26</sup> package defines both `\D` and `\E`, for example). In order to give you control which commands are defined in which way, there is the package option `iupac`. It has three modes:

- `iupac` = auto: if the commands are *not* defined by any package or class you're using they are available generally, otherwise only *inside* `\iupac`.

<sup>24</sup> The idea and the implementation is shamelessly borrowed from bpchem by Bjørn Pedersen. <sup>25</sup> Actually another mechanism is used, but the effect is essentially the same. <sup>26</sup> CTAN: `cool`

- `iupac` = restricted: all naming commands are *only* defined inside `\iupac`. If the commands are defined by another package they of course have that meaning outside. They're not defined outside otherwise.
- `iupac` = strict: `CHEMMACROS` overwrites any other definition and makes the commands available throughout the document. Of course the commands can be redefined (but only in the document body). They will still be available inside `\iupac` then.

Table 2 demonstrates the different modes.

Table 2: Demonstration of `iupac`'s modes.

	auto	restricted	strict
<code>\L</code>	L̸	L̸	L
<code>\iupac{\L}</code>	L	L	L
<code>\D</code>	D	–	D
<code>\iupac{\D}</code>	D	D	D

### 9.1.1. Predefined Commands

The macros in this section are intended to make the writing of IUPAC names more convenient.

**Greek Letters** Greek letters in compound names are typeset upright. For this there are the packages `upgreek` and `textgreek`. If you have loaded one of them `CHEMMACROS` typesets the following commands upright:

- `\a` →  $\alpha$
- `\b` →  $\beta$
- `\g` →  $\gamma$
- `\d` →  $\delta$
- `\k` →  $\kappa$
- `\m` →  $\mu$
- `\n` →  $\eta$
- `\w` →  $\omega$

```

1 \iupac{5\a-androstan-3\b-ol} \
2 \iupac{\a-(tri\|chloro\|methyl)\-\w-chloro\|poly(1,4-phenylene\|methylene)}

5 $\alpha$ -androstan-3 $\beta$ -ol
 $\alpha$ -(trichloromethyl)- $\omega$ -chloropoly(1,4-phenylenemethylene)

```

**Hetero Atoms and added Hydrogen** Attachments to hetero atoms and added hydrogen atoms are indicated by italic letters [[Coh+o8](#)]. [CHEMMACROS](#) defines a few shortcuts for the most common ones.

- ▶ `\H` → *H*
- ▶ `\O` → *O*
- ▶ `\N` → *N*
- ▶ `\Sf` → *S*
- ▶ `\P` → *P*

1	<code>\iupac{\N-methyl\benz\amide} \</code>	<i>N</i> -methylbenzamide
2	<code>\iupac{3\H-pyrrole} \</code>	<i>3H</i> -pyrrole
3	<code>\iupac{\O-ethyl hexanethioate}</code>	<i>O</i> -ethyl hexanethioate

### Cahn-Ingold-Prelog

- ▶ `\cip{<conf>}` → e.g.: `\cip{R,S}` (*R,S*)
- ▶ `\R` → (*R*)
- ▶ `\S` → (*S*)

Since the command `\S` has another meaning already ( $\S$ ) it is only available inside `\iupac` in the default setting.

Both these commands and the entgegen/zusammen descriptors get a small additional amount of kerning after the closing parenthesis. This amount can be changed through the following option:

`iupac` ▶ `cip-kern` = <dim> → amount of kerning after the closing parenthesis. Default = .1ex

### Fischer

- ▶ `\D` → *D*
- ▶ `\L` → *L*

Since the command `\L` has another meaning already ( $\mathbb{L}$ ) it is only available inside `\iupac` in the default setting.

### cis/trans, zusammen/entgegen, syn/anti & tert

- ▶ `\cis` → *cis*
- ▶ `\trans` → *trans*
- ▶ `\Z` → (*Z*)
- ▶ `\E` → (*E*)

► `\syn` → *syn*

► `\anti` → *anti*

► `\tert` → *tert*

The package `cool` defines the commands `\E` and `\D`, too. If you load it, the `CHEMMACROS` version will only be available inside `\iupac` in the default setting.

### ortho/meta/para

► `\ortho` → *o*

► `\meta` → *m*

► `\para` → *p*

### Absolute Configuration (uses TikZ)

► `\Rconf[<letter>]` → `\Rconf:`  `\Rconf[]:` 

► `\Sconf[<letter>]` → `\Sconf:`  `\Sconf[]:` 

Examples:

```
1 \iupac{\D\Wein\|s\"aure} = \\
2 \iupac{\cip{2S,3S}\Wein\|s\"aure} \\
3 \iupac{\D\-(\$-\$)\-Threose} = \\
4 \iupac{\cip{2S,3R}\-(\$-\$)\-2,3,4-Tri\|hydroxy\|butanal} \\
5 \iupac{\cis\2\Butene} = \\
6 \iupac{\Z\2\Butene}, \\
7 \iupac{\cip{2E,4Z}\Hexa\|diene} \\
8 \iupac{\meta\Xylol} = \\
9 \iupac{1,3-Di\|methyl\|benzene}
```

D-Weinsäure =  
(2*S*,3*S*)-Weinsäure  
D-(–)-Threose =  
(2*S*,3*R*)-(–)-2,3,4-Trihydroxybutanal  
*cis*-2-Butene =  
(*Z*)-2-Butene,  
(2*E*,4*Z*)-Hexadiene  
*m*-Xylol =  
1,3-Dimethylbenzene

**Coordination Chemistry** `CHEMMACROS` provides two commands useful with coordination chemistry:

► `\bridge{<num>}` →  $\mu_3$ -

► `\hapto{<num>}` →  $\eta^5$ -

```

1 Ferrocene = \iupac{bis(\hapto{5}cyclo\penta\dienyl)iron} \
2 \iupac{tetra-\bridge{3}iodido-tetrakis[tri\methyl\platinum(IV)]}

```

Ferrocene = bis( $\eta^5$ -cyclopentadienyl)iron  
tetra- $\mu_3$ -iodido-tetrakis[trimethylplatinum(IV)]

Two options allow customization:

**iupac** ► **bridge-number** = sub|super → appends the number as a subscript or superscript. IUPAC recommendation is the subscript [Con+05]. Default = sub

**iupac** ► **coord-use-hyphen** = true|false → append a hyphen to \hapto and \bridge or don't. Default = true

### 9.1.2. Own Naming Commands

If you find any commands missing you can define them using

► \DeclareChemIUPAC{<cmd>} → {<declaration>}

► \RenewChemIUPAC{<cmd>} → {<declaration>}

A command defined in this way will obey the setting of the option **iupac**. This means any existing command is only overwritten with **iupac** = strict. However, \DeclareChemIUPAC will *not* change the definition of an existing IUPAC naming command but issue a warning/an error (depending on the package option **strict**) if the IUPAC naming command already exists.

```

1 \DeclareChemIUPAC\endo{\textit{endo}}
2 \RenewChemIUPAC\anti{\textit{anti}}
3 \iupac{(2-\endo,7-\anti)-2-bromo-7-fluoro\bicyclo[2.2.1]heptane}

(2-endo,7-anti)-2-bromo-7-fluorobicyclo[2.2.1]heptane

```

\RenewChemIUPAC allows you to redefine the existing IUPAC naming commands.

1 \iupac{\meta-Xylol} \	<i>m</i> -Xylol
2 \RenewChemIUPAC\meta{\textit{m}}	<i>m</i> -Xylol
3 \iupac{\meta-Xylol}	

### 9.2. Latin Phrases

The package chemstyle provides the command \latin to typeset common latin phrases in a consistent way. CHEMMACROS defines a similar \latin only if chemstyle has *not* been loaded and additionally provides these commands:

► \insitu → *in situ*

► \abinitio → *ab initio*

► \invacuo → *in vacuo*



## 10. Units for the Usage With siunitx

If the package chemstyle has been loaded they are defined using chemstyle's `\latin` command. This means that then the appearance depends on chemstyle's option `abbremp`:

1	<code>\insitu, \abinitio\</code>	<i>in situ, ab initio</i>
2	<code>\cstsetup{abbremp=false}</code>	in situ, ab initio
3	<code>\insitu, \abinitio</code>	

The commands are defined through

- ▶ `\DeclareChemLatin{<cmd>}{<phrase>}`
- ▶ `\RenewChemLatin{<cmd>}{<phrase>}`

1	<code>\DeclareChemLatin\ltn{latin text}</code>	<i>latin text latin text</i>
2	<code>\ltn \cstsetup{abbremp=false} \ltn</code>	

If you have *not* loaded chemstyle you can change the appearance with this option:

`latin` ▶ `format` = <definition> → Default = `\itshape`

## 10. Units for the Usage With siunitx

In chemistry some non-SI units are very common. siunitx provides the command `\DeclareSIUnit{<command>}{<unit>}` to add arbitrary units. CHEMMACROS uses that command to provide some units. Like all siunitx units they're only valid inside `\SI{<num>}{<unit>}` and `\si{<unit>}`.

- ▶ `\atmosphere` → atm
- ▶ `\atm` → atm
- ▶ `\calory` → cal
- ▶ `\cal` → cal
- ▶ `\cmc` → cm<sup>3</sup> The units `\cmc`, `\molar`, and `\Molar` are defined by the package chemstyle as well. CHEMMACROS only defines them, if chemstyle is not loaded.
- ▶ `\molar` → mol dm<sup>-3</sup>
- ▶ `\moLar` → mol L<sup>-1</sup>
- ▶ `\Molar` → M
- ▶ `\MolMass` → g mol<sup>-1</sup>
- ▶ `\normal` → N
- ▶ `\torr` → torr

By the way: `\mmHg` mmHg already is defined by siunitx and chemstyle

## 11. Acid/Base

Easy representation of pH,  $pK_A$  ... (the command `\pKa` depends on the package option `language`).

- ▶ `\pH` → pH
- ▶ `\pOH` → pOH
- ▶ `\Ka` →  $K_A$
- ▶ `\Kb` →  $K_B$
- ▶ `\Kw` →  $K_W$
- ▶ `\pKa[<num>]` → `\pKa:`  $pK_A$ , `\pKa[1]:`  $pK_{A1}$
- ▶ `\pKb[<num>]` → `\pKb:`  $pK_B$ , `\pKb[1]:`  $pK_{B1}$
- ▶ `\p{<anything>}` → e.g. `\p{\Kw}`  $pK_W$

<code>\Ka \Kb \pKa \pKa[1] \pKb \pKb[1]</code>	$K_A \ K_B \ pK_A \ pK_{A1} \ pK_B \ pK_{B1}$
--	---

The default appearance of the p-commands has changed to follow IUPAC recommendations.

The operator p [...] shall be printed in Roman type. *IUPAC Green Book [Coh+08, p. 103]*

There is one option which changes the style the p is typeset:

`acid-base` ▶ `p-style` = `italics|slanted|upright` → Default = `upright`

<pre> 1 \pH, \pKa 2 3 \chemsetup[acid-base]{p-style=slanted} \pH, \pKa 4 5 \chemsetup[acid-base]{p-style=italics} \pH, \pKa </pre> <p> <math>pH, pK_A</math>  <math>pH, pK_A</math>  <math>pH, pK_A</math> </p>
---

## 12. Oxidation Numbers, Real and Formal Charges

`CHEMMACROS` distinguishes between real (+/−) and formal ( $\oplus/\ominus$ ) charge symbols, also see section 4. All commands using formal charge symbols start with a f.

## 12.1. Ion Charges

Simple displaying of (real) charges:

- `\pch[<number>]` → positive charge (plus + charge)
- `\mch[<number>]` → negative charge (minus + charge)

1	<code>\pch</code> , <code>Na\pch</code> , <code>Ca\pch[2]\</code>	$^+$ , $\text{Na}^+$ , $\text{Ca}^{2+}$
2	<code>\mch</code> , <code>F\mch</code> , <code>S\mch[2]</code>	$^-$ , $\text{F}^-$ , $\text{S}^{2-}$

The same for formal charges:

- `\fpch[<number>]` → positive charge
- `\fmch[<number>]` → negative charge

1	<code>\fpch</code> <code>\fmch</code> <code>\fpch[3]</code> <code>\fmch[3]</code>	$\oplus$ $\ominus$ $3\oplus$ $3\ominus$
---	---	---

There is a key which influences the behaviour of the charges.

`charges` ► `append` = `true`|`false` → if set true, the charge is appended together with an empty group.

This is how the key influences the behaviour:

1	% uses package 'mhchem'
2	<code>\chemsetup{charges/append=false,phases/pos=sub}</code>
3	<code>\ce{H\pch\aq}</code> <code>\ce{H\aq\pch}</code>
4	
5	<code>\chemsetup[charges]{append=true}</code>
6	<code>\ce{H\pch\aq}</code> <code>\ce{H\aq\pch}</code>
$\text{H}_{(\text{aq})}^+ \text{H}_{(\text{aq})}^+$ $\text{H}_{(\text{aq})}^+ \text{H}_{(\text{aq})}^+$	

In most cases this behaviour will be unwanted. However, in some cases it might be useful, for example together with the `\ox` command (see next section):

1	<code>\chemsetup{charges/append=false,phases/pos=sub}</code>
2	<code>\ce{\ox{1,H}\pch\aq}</code>
3	
4	<code>\chemsetup[charges]{append=true}</code>
5	<code>\ce{\ox{1,H}\pch\aq}</code>
$\text{H}_{(\text{aq})}^+$ $\text{H}_{(\text{aq})}^+$	

## 12.2. Oxidation Numbers

Typesetting oxidation numbers:

- `\ox[<keyval>]{<number>,<atom>}` → places <number> above <atom>; <number> has to be a (rational) number!

```
1 \ox{+1,Na}, \ox{2,Ca}, \ox{-2,S}, \ox{-1,F}      Na, Ca, S, F
```

There are a number of keys, that can be used to modify the `\ox` command.

- `\ox` ► `parse` = `true`|`false` → when `false` an arbitrary entry can be used for <number>. Default = `true`
- `\ox` ► `roman` = `true`|`false` → switches from roman to arabic numbers. Default = `true`
- `\ox` ► `pos` = `top`|`super`|`side` →; `top` places <number> above <atom>, `super` to the upper right as superscript and `side` to the right and inside brackets. Default = `top`
- `\ox` ► `explicit-sign` = `true`|`false` → shows the + for positiv numbers and the ± for 0. Default = `false`
- `\ox` ► `decimal-marker` = `comma`|`point` → choice for the decimal marker for formal oxidation numbers like  $\overset{1.2}{X}$ . Default = `point`
- `\ox` ► `align` = `center`|`right` → center the oxidation number relative to the atom or right-align it. Default = `center`

```
1 \ox[roman=false]{2,Ca} \ox{2,Ca} \ \           Ca Ca
2 \ox[pos=super]{3,Fe}-Oxide \ \               FeIII-Oxide
3 \ox[pos=side]{3,Fe}-Oxide \ \               Fe(III)-Oxide
4 \ox[parse=false]{?,Mn} \ \                  ?
5 \ox[align=right]{2,Ca}                      Mn
                                              Ca
```

The `pos = super` variant also can be set with the shortcut `\ox*`:

```
1 \ox{3,Fe} \ox*{3,Fe}                        Fe FeIII
```

Using the `explicit-sign` key will always show the sign of the oxidation number:

```
1 \chemsetup[ox]{explicit-sign = true}
2 \ox{+1,Na}, \ox{2,Ca}, \ox{-2,S}, \ch{"\ox{0,F}" {2}}

+INa, +IICa, -II±0S, F2
```

```
1 Compare \ox{-1,\ch{O2^2-}} to \ch{"\ox{-1,O}" {2}^2-}

Compare O2-I to O2-I
```

## 12. Oxidation Numbers, Real and Formal Charges

Sometimes one might want to use formal oxidation numbers like 0.5 or  $\frac{1}{3}$ :

```
1 \ox{.5,\ch{Br2}} \ch{"\ox{1/3,I}" {}3+}  $\text{Br}_2 \text{I}_3^{+}$ 
```

The fraction uses the `\sfrac` command of the `xfrac`<sup>27</sup> package. For this purpose the instance `chemmacros-ox-frac` is defined.

```
1 \DeclareInstance{xfrac}{chemmacros-ox-frac}{text}
2 {
3   scale-factor      = 1.2 ,
4   denominator-bot-sep = -.5ex ,
5   numerator-top-sep  = -.3ex ,
6   slash-left-kern    = -.2em ,
7   slash-right-kern   = -.2em ,
8   slash-symbol-font  = lmr
9 }
```

Of course you can redefine it so that it suits your needs as the output often strongly depends on the used font.

### 12.3. Partial Charges and Similar Stuff

The next ones probably are seldomly needed but nevertheless useful:

- `\delp` →  $\delta+$  (delta + plus)
- `\delm` →  $\delta-$  (delta + minus)
- `\fdelp` →  $\delta\oplus$
- `\fdelm` →  $\delta\ominus$

These macros for example can be used with the `\ox` command or with the `chemfig` package:

```
1 \chemsetup{
2   option/circled = all,
3   ox/parse      = false
4 }
5 \ce{\ox{\delp,H}-\ox{\delm,Cl}} \hspace*{1cm}
6 \chemfig{\chemabove[3pt]{\lewis{246,Br}}{\delm}-\chemabove[3pt]{H}{\delp}}
```

$$\begin{array}{ccc} \delta\oplus & \delta\ominus & \delta\ominus & \delta\oplus \\ \text{H} - \text{Cl} & & |\text{Br} - \text{H} \end{array}$$

The following macros are useful together with `chemfig`, too.

- `\scrip` → + (scriptstyle + plus)
- `\scrim` → − (scriptstyle + minus)
- `\fscrip` →  $\oplus$

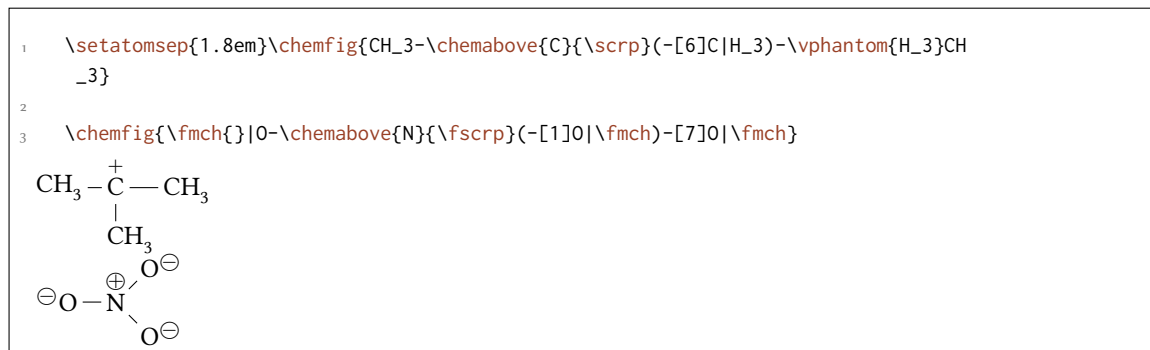
---

<sup>27</sup> CTAN: `xfrac`

► `\fscrm` →  $\ominus$

► `\fsscrp` →  $\oplus$  (using `\scriptscriptstyle`)

► `\fsscrm` →  $\ominus$



## 13. Reaction Mechanisms

With the command

► `\mech[<type>]`

one can specify the most common reaction mechanisms. `<type>` can have one of the following values:

► `\mech` → (empty, no opt. argument) nucleophilic substitution  $S_N$

► `\mech[1]` → unimolecular nucleophilic substitution  $S_{N1}$

► `\mech[2]` → bimolecular nucleophilic substitution  $S_{N2}$

► `\mech[se]` → electrophilic substitution  $S_E$

► `\mech[1e]` → unimolecular electrophilic substitution  $S_{E1}$

► `\mech[2e]` → bimolecular electrophilic substitution  $S_{E2}$

► `\mech[ar]` → electrophilic aromatic substitution  $Ar-S_E$

► `\mech[e]` → elimination  $E$

► `\mech[e1]` → unimolecular elimination  $E_1$

► `\mech[e2]` → bimolecular elimination  $E_2$

► `\mech[cb]` → unimolecular elimination “conjugated base”, i.e. via carbanion  $E_{1cb}$

## 14. Redox Reactions

**CHEMMACROS** provides two commands to visualize the transfer of electrons in redox reactions. Both commands are using **TikZ**.

- `\OX{<name>,<atom>}`
- `\redox(<name1>,<name2>)[<tikz>][<num>]<text>` → Only the first argument (<name1>,<name2>) is required, the others are all optional.

`\OX` places <atom> into a node, which is named with <name>. If you have set two `\OX`, they can be connected with a line using `\redox`. To do so the names of the two nodes that are to be connected are written in the round braces. Since `\redox` draws a `tikzpicture` with options `remember picture, overlay`, the document needs to be *compiled at least two times*.

```
1 \OX{a,Na} $\rightarrow$ \OX{b,Na}\pch\redox(a,b){oxidation}
   oxidation
   ┌───┐
   │   │
Na → Na+
```

This line can be customized using **TikZ** keys in [<tikz>]:

```
1 \OX{a,Na} $\rightarrow$ \OX{b,Na}\pch\redox(a,b)[->,red]{ox}
```

With the argument [<num>] the length of the vertical parts of the line can be adjusted. The default length is .6em. This length is multiplied with <num>. If you use a negative value the line is placed *below* the text.

```
1 \OX{a,Na} $\rightarrow$ \OX{b,Na}\pch
2 \redox(a,b)[->,red]{ox}
3 \redox(a,b)[<-,blue][-1]{red}
4 \vspace{7mm}
   ox
   ┌───┐
   │   │
Na → Na+
   └───┘
   red
```

The default length of the vertical lines can be customized with the option

`\redox` ► `dist = <dim>` → A  $\text{\TeX}$  dimension. Default = .6em

```
1 \chemsetup{redox/dist=1em}
2 \OX{a,Na} $\rightarrow$ \OX{b,Na}\pch\redox(a,b)[->,red]{ox}
   ox
   ┌───┐
   │   │
Na → Na+
```

Additionally the option

`\redox` ► `sep = <dim>` → Default = .2em

can be used to change the distance between the atom and the beginning of the line.

## 14. Redox Reactions

```

1 \chemsetup{redox/sep=.5em}
2 \OX{a,Na} $\rightarrow$ \OX{b,Na}\pch\redox(a,b)[->,red]{ox}

```

OX

$\text{Na} \rightarrow \text{Na}^+$

Examples:

```

1 \ch{ 2 "\OX{o1,Na}" + "\OX{r1,Cl}" {}2 -> 2 "\OX{o2,Na}" \pch{} + 2
2 "\OX{r2,Cl}" \mch {}
3 \redox(o1,o2){\small OX: $- 2\text{el}$}
4 \redox(r1,r2){\small RED: $+ 2\text{el}$}
5 \vspace{7mm}

```

OX:  $-2e^-$

$2 \text{Na} + \text{Cl}_2 \rightarrow 2 \text{Na}^+ + 2 \text{Cl}^-$

RED:  $+2e^-$

```

1 \ch{ 2 "\OX{o1,\ox{0,Na}}" + "\OX{r1,\ox{0,Cl}}" {}2 -> 2 "\OX{o2,\ox{+1,Na}}"
2 \pch{} + 2 "\OX{r2,\ox{-1,Cl}}" \mch {}
3 \redox(o1,o2){\small OX: $- 2\text{el}$}
4 \redox(r1,r2){\small RED: $+ 2\text{el}$}
5 \vspace{7mm}

```

OX:  $-2e^-$

$2 \text{Na} + \text{Cl}_2 \rightarrow 2 \text{Na}^+ + 2 \text{Cl}^-$

RED:  $+2e^-$

```

1 \ch{ 2 "\OX{o1,\ox{0,Na}}" + "\OX{r1,\ox{0,Cl}}" {}2 -> 2 "\OX{o2,\ox{+1,Na}}"
2 \pch{} + 2 "\OX{r2,\ox{-1,Cl}}" \mch {}
3 \redox(o1,o2)[draw=red,->][3.33]{\small OX: $- 2\text{el}$}
4 \redox(r1,r2)[draw=blue,->]{\small RED: $+ 2\text{el}$}

```

OX:  $-2e^-$

$2 \text{Na} + \text{Cl}_2 \rightarrow 2 \text{Na}^+ + 2 \text{Cl}^-$

RED:  $+2e^-$



```

1 \ch{ 2 "\OX{o1,\ox{0,Na}}" + "\OX{r1,\ox{0,Cl}}" {}2 -> 2 "\OX{o2,\ox{+1,Na}}"
2 \pch{} + 2 "\OX{r2,\ox{-1,Cl}}" \mch {}
3 \redox{o1,o2}[green,-stealth]{\small OX}
4 \redox{r1,r2}[purple,-stealth][-1]{\small RED}
5 \vspace{7mm}

```

$$2 \overset{0}{\text{Na}} + \overset{0}{\text{Cl}}_2 \rightarrow 2 \overset{+1}{\text{Na}} + 2 \overset{-1}{\text{Cl}}$$

## 15. (Standard) State, Thermodynamics

### 15.1. Thermodynamic Variables

The following commands use siunitx:

- `\Enthalpy[<keyval>](<subscript>){<value>}`
- `\Entropy[<keyval>](<subscript>){<value>}`
- `\Gibbs[<keyval>](<subscript>){<value>}`

Their usage is pretty much self-explaining:

1	<code>\Enthalpy{123} \\\</code>	$\Delta H^\ominus = 123 \text{ kJ mol}^{-1}$
2	<code>\Entropy{123} \\\</code>	$S^\ominus = 123 \text{ J K}^{-1} \text{ mol}^{-1}$
3	<code>\Gibbs{123}</code>	$\Delta G^\ominus = 123 \text{ kJ mol}^{-1}$

The argument (`<subscript>`) adds a subscript for specification: `\Enthalpy(r){123}`  $\Delta_r H^\ominus = 123 \text{ kJ mol}^{-1}$ .

There are several keys to customize the commands.

- none- ► `exponent` = `<anything>`
- none- ► `delta` = `<anything>|false`
- none- ► `subscript` = `left|right`
- none- ► `unit` = `<unit>`

The default values depend on the command.

1	<code>\Enthalpy[unit=\kilo\joule]{-285} \\\</code>	$\Delta H^\ominus = -285 \text{ kJ}$
2	<code>\Gibbs[delta=false]{0} \\\</code>	$G^\ominus = 0 \text{ kJ mol}^{-1}$
3	<code>\Entropy[delta=\Delta,exponent=]{56.7}</code>	$\Delta S = 56.7 \text{ J K}^{-1} \text{ mol}^{-1}$

The unit is set corresponding to the rules of siunitx and depends on its settings:

```

1 \Enthalpy{-1234.56e3} \\
2 \sisetup{per-mode=symbol,exponent-product=\cdot,output-decimal-marker={,},group-
   four-digits=true}
3 \Enthalpy{-1234.56e3}


$$\Delta H^\ominus = -1234.56 \times 10^3 \text{ kJ mol}^{-1}$$


$$\Delta H^\ominus = -1\,234,56 \cdot 10^3 \text{ kJ/mol}$$


```

### 15.1.1. Create New Variables

You can use the command

► `\DeclareChemState[<keyval>]{<name>}{<symbol>}{<unit>}`

to create new corresponding commands:

```

1 \DeclareChemState{Helmholtz}{A}{\kilo\joule\per\mole}
2 \DeclareChemState[subscript-left=false,exponent=]{ElPot}{E}{\volt}
3 \Helmholtz{123.4} \\
4 \ElPot{-1.1} \\
5 \ElPot[exponent=0]{$\ch{Sn}|\ch{Sn^2+}||\ch{Pb^2+}|\ch{Pb}}{0.01}


$$\Delta A^\ominus = 123.4 \text{ kJ mol}^{-1}$$


$$\Delta E = -1.1 \text{ V}$$


$$\Delta E_{\text{Sn}|\text{Sn}^{2+}||\text{Pb}^{2+}|\text{Pb}}^0 = 0.01 \text{ V}$$


```

The command has some keys with which the default behaviour of the new command can be set.

► `exponent` = <anything>

► `delta` = <anything>|false

~~►~~ `subscript-left` = true|false

► `subscript` = <anything>

### 15.1.2. Redefine Variables

With

► `\RenewChemState[<keyval>]{<name>}{<symbol>}{<unit>}`

you can redefine the already existing commands:

```

1 \RenewChemState{Enthalpy}{h}{\joule}
2 \Enthalpy(f){12.5}


$$\Delta_f h^\ominus = 12.5 \text{ J}$$


```

The command is analogous to `\DeclareChemState`, i.e. it has the same keys.

So – for following thermodynamic conventions – one could define a molar and an absolute variable:

```

1 \DeclareChemState[exponent=]{enthalpy}{h}{\kilo\joule\per\mole}% molar
2 \RenewChemState[exponent=]{Enthalpy}{H}{\kilo\joule}% absolute
3 \enthalpy{-12.3} \Enthalpy{-12.3}


$$\Delta h = -12.3 \text{ kJ mol}^{-1} \quad \Delta H = -12.3 \text{ kJ}$$


```

## 15.2. State

The commands presented in section 15.1 internally all use the command<sup>28</sup>

► `\State[<keyval>]{<symbol>}{<subscript>}`

It can be used to write the thermodynamic variables without value and unit.

Examples:

```

1 \State{A}, \State{G}{f}, \State[subscript-left=false]{E}{\ch{Na}}, \State[
  exponent=\SI{1000}{\celsius}]{H}


$$\Delta A^\ominus, \Delta_f G^\ominus, \Delta E_{\text{Na}}^\ominus, \Delta H^{1000^\circ\text{C}}$$


```

Again there are some keys to customize the command:

`state` ► `exponent` = <anything>

`state` ► `subscript-left` = `true`|`false`

`state` ► `delta` = <anything>|`false`

## 16. Spectroscopy and Experimental Data

### 16.1. The `\NMR` Command

When you're trying to find out if a compound is the one you think it is often NMR spectroscopy is used. The experimental data are typeset similar to this:

<sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>):  $\delta = 1.59$

`CHEMMACROS` provides a command which simplifies the input (uses `siunitx`).

► `\NMR*{<num>,<elem>}{<num>,<unit>}[<solvent>]`

All Argument are optional! Without arguments we get:

```

1 \NMR \ \ 1H-NMR:  $\delta$ 
2 \NMR* 1H-NMR

```

The first argument specifies the kind of NMR:

<sup>28</sup> Please note that `{<subscript>}` is an *optional* argument.

1 \NMR{13,C}	<sup>13</sup> C-NMR: $\delta$
--------------	-------------------------------

The second argument sets the frequency (in MHz):

1 \NMR(400)	<sup>1</sup> H-NMR (400 MHz): $\delta$
-------------	--

You can choose another unit:

1 \NMR(4e8,\hertz)	<sup>1</sup> H-NMR ( $4 \times 10^8$ Hz): $\delta$
--------------------	--

Please note that the setup of siunitx also affects this command:

1 \sisetup{exponent-product=\cdot}\NMR(4e8,\hertz)	<sup>1</sup> H-NMR ( $4 \cdot 10^8$ Hz): $\delta$
--	---

The third argument specifies the solvent:

1 \NMR[CDCl3]	<sup>1</sup> H-NMR (CDCl <sub>3</sub> ): $\delta$
---------------	---

## 16.2. Short Cuts

It is possible to define short cut commands for specific nuclei.

- \DeclareChemNMR{<csname>}{<num>,<atom>}
- \RenewChemNMR{<csname>}{<num>,<atom>}

This defines a command with the same arguments as \NMR *except* for {<num>,<atom>}.

1 \DeclareChemNMR\HNMR{1,H}%	<sup>13</sup> C-NMR (100 MHz)
2 \DeclareChemNMR\CNMR{13,C}%	<sup>1</sup> H-NMR (400 MHz)
3 \CNMR*(100) \	
4 \HNMR*(400)	

## 16.3. An Environment to Typeset Experimental Data

CHEMMACROS provides an environment to ease the input of experimental data.

- \begin{experimental} data \end{experimental} → Environment for the output of experimental data. Inside the environment the following commands are defined.
- \data{<type>}[<specification>] → Type of data, e.g. IR, MS... The optional argument takes further specifications which are output in parentheses.
- \data\*{<type>}[<specification>] → Like \data but changes the = into a :, given that use-equal = true is used.

- ▶ `\NMR{<num>,<elem>[<coupling core>]}(<num>,<unit>)[<solvent>]` → this command gets an additional argument: `\NMR{13,C[^1H]} 13C{1H}-NMR:  $\delta$`
- ▶ `\J(<bonds>;<nuclei>)[<unit>]{<list of nums>}` → Coupling constant, values are input separated by ; (NMR). The argument (<bonds>;<nuclei>) is optional and enables further specifications of the coupling.
- ▶ `\#{<num>}` → Number of nuclei (NMR).
- ▶ `\pos{<num>}` → Position of nuclues (NMR).
- ▶ `\val{<num>}` → A number, an alias of siunitx' `\num{<num>}`
- ▶ `\val{<num1>--<num2>}` → An alias of siunitx' `\numrange{<num1>}{<num2>}`

```

1 \begin{experimental}
2   \data{type1} Data.
3   \data{type2}[specifications] More data.
4   \data*{type3} Even more data.
5 \end{experimental}

```

type1 Data. type2 (specifications) More data. type3  
Even more data.

#### 16.4. Customization

The output of the environment and of the NMR commands can be customized by a number of options. For historical reasons they all belong to the module `nmr`.

- `nmr` ▶ `unit` = <unit> → Default = `\mega\hertz`
- `nmr` ▶ `nucleus` = {<num>,<atom>} → Default = {1,H}
- `nmr` ▶ `format` = <commands> → for example `\bfseries`
- `nmr` ▶ `pos-number` = side|sub → Position of the number next to the atom. Default = side
- `nmr` ▶ `coupling-unit` = <unit> → A siunitx unit. Default = `\hertz`
- `nmr` ▶ `parse` = `true`|false → Treat the solvent as mhchem/`CHEMFORMULA` formula or not. Default = `true`
- `nmr` ▶ `delta` = <tokens> → The <tokens> are added after  $\delta$ .
- `nmr` ▶ `list` = `true`|false → The environment `\begin{nmr}[<optionen>] \end{nmr}` is formatted as a list. Default = false
- `nmr` ▶ `list-setup` = <setup> → Setup of the list. Default = see below.
- `nmr` ▶ `use-equal` = `true`|false → Add equal sign after `\NMR` and `\data`. Default = false

The default setup of the list:

```

1 \topsep\z@skip \partopsep\z@skip
2 \itemsep\z@ \parsep\z@ \itemindent\z@
3 \leftmargin\z@

```

```

1 \begin{experimental}[format=\bfseries]
2 \data{type1} Data.
3 \data{type2}[specifications] More data.
4 \data*{type3} Even more data.
5 \end{experimental}

```

type1 Data. type2 (specifications) More data.  
type3 Even more data.

The command `\NMR` and all commands defined through `\DeclareChemNMR` can be used like `\data` for the NMR data.

```

1 \begin{experimental}[format=\bfseries,use-equal]
2 \data{type1} Data.
3 \data{type2}[specifications] More data.
4 \NMR Even more data.
5 \end{experimental}

```

type1 = Data. type2 (specifications) = More data. <sup>1</sup>H-NMR:  $\delta$  = Even more data.

### 16.5. An Example

The code below is shown with different specifications for `<optionen>`. Of course options can also be chosen with `\chemsetup`.

```

1 \sisetup{separate-uncertainty,per-mode=symbol,detect-all,range-phrase=--}
2 \begin{experimental}[<optionen>]
3 \data*{yield} \SI{17}{\milli\gram} yellow needles (\SI{0.04}{\milli\mole}, \
4 \SI{13}{\percent}).
5 %
6 \data{mp.} \SI{277}{\celsius} (DSC).
7 %
8 \NMR(600)[CDC13] \val{2.01} (s, \#{24}, \pos{5}), \val{2.31} (s, \#{12}, \
9 \pos{1}), \val{6.72--6.74} (m, \#{2}, \pos{11}), \val{6.82} (s, \#{8}, \pos
10 {3}), \val{7.05--7.07} (m, \#{2}, \pos{12}), \val{7.39--7.41} (m, \#{4}, \
11 \pos{9}), \val{7.48--7.49} (m, \#{4}, \pos{8}).
12 %
13 \NMR{13,C}(150)[CDC13] \val{21.2} ($+$, \#{4}, \pos{1}), \val{23.4} ($+$,
14 \#{8}, \pos{5}), \val{126.0} ($+$, \#{4}, \pos{9}), \val{128.2} ($+$,
15 \#{8}, \pos{3}), \val{130.8} ($+$, \#{2}, \pos{12}), \val{133.6} ($+$,
16 \#{2}, \pos{11}), \val{137.0} ($+$, \#{4}, \pos{8}), \val{138.6} (q, \#{4},
17 \pos{2}), \val{140.6} (q, \#{2}, \pos{10}), \val{140.8} (q, \#{8}, \pos
18 {4}), \val{141.8} (q, \#{4}, \pos{6}), \val{145.6} (q, \#{2}, \pos{7}).
19 %
20 \data{MS}[DCP, EI, \SI{60}{\electronvolt}] \val{703} (2, \ch{M+}), \val{582}
21 (1), \val{462} (1), \val{249} (13), \val{120} (41), \val{105} (100).
22 %
23 \data{MS}[\ch{MeOH + H2O + KI}, ESI, \SI{10}{\electronvolt}] \val{720} (100,

```

```

\ch{M+ + OH-}), \val{368} (\ch{M+ + 2 OH-}).
14 %
15 \data{IR}[KBr] \val{3443} (w), \val{3061} (w), \val{2957} (m), \val{2918} (m
), \val{2856} (w), \val{2729} (w), \val{1725} (w), \val{1606} (s), \val
{1592} (s), \val{1545} (w), \val{1446} (m), \val{1421} (m), \val{1402} (m),
\val{1357} (w), \val{1278} (w), \val{1238} (s), \val{1214} (s), \val{1172}
(s), \val{1154} (m), \val{1101} (w), \val{1030} (w), \val{979} (m), \val
{874} (m), \val{846} (s), \val{818} (w), \val{798} (m), \val{744} (w), \val
{724} (m), \val{663} (w), \val{586} (w), \val{562} (w), \val{515} (w).
16 %
17 \data*{UV-Vis} \SI{386}{\nano\metre} ($\varepsilon = \val{65984}$), \SI
{406}{\nano\metre} ($\varepsilon = \val{65378}$).
18 %
19 \data*{quantum yield} $\Phi = \val{0.74+-0.1}$, .
20 \end{experimental}

```

### 16.5.1. Nearly Standard

Output with these options: <optionen>: delta=(ppm),pos-number=sub,use-equal

yield: 17 mg yellow needles (0.04 mmol, 13 %). mp. = 277 °C (DSC). <sup>1</sup>H-NMR (600 MHz, CDCl<sub>3</sub>): δ (ppm) = 2.01 (s, 24 H, H<sub>5</sub>), 2.31 (s, 12 H, H<sub>1</sub>), 6.72–6.74 (m, 2 H, H<sub>11</sub>), 6.82 (s, 8 H, H<sub>3</sub>), 7.05–7.07 (m, 2 H, H<sub>12</sub>), 7.39–7.41 (m, 4 H, H<sub>9</sub>), 7.48–7.49 (m, 4 H, H<sub>8</sub>). <sup>13</sup>C-NMR (150 MHz, CDCl<sub>3</sub>): δ (ppm) = 21.2 (+, 4 C, C<sub>1</sub>), 23.4 (+, 8 C, C<sub>5</sub>), 126.0 (+, 4 C, C<sub>9</sub>), 128.2 (+, 8 C, C<sub>3</sub>), 130.8 (+, 2 C, C<sub>12</sub>), 133.6 (+, 2 C, C<sub>11</sub>), 137.0 (+, 4 C, C<sub>8</sub>), 138.6 (q, 4 C, C<sub>2</sub>), 140.6 (q, 2 C, C<sub>10</sub>), 140.8 (q, 8 C, C<sub>4</sub>), 141.8 (q, 4 C, C<sub>6</sub>), 145.6 (q, 2 C, C<sub>7</sub>). MS (DCP, EI, 60 eV) = 703 (2, M<sup>+</sup>), 582 (1), 462 (1), 249 (13), 120 (41), 105 (100). MS (MeOH + H<sub>2</sub>O + KI, ESI, 10 eV) = 720 (100, M<sup>+</sup> + OH<sup>-</sup>), 368 (M<sup>+</sup> + 2 OH<sup>-</sup>). IR (KBr) = 3443 (w), 3061 (w), 2957 (m), 2918 (m), 2856 (w), 2729 (w), 1725 (w), 1606 (s), 1592 (s), 1545 (w), 1446 (m), 1421 (m), 1402 (m), 1357 (w), 1278 (w), 1238 (s), 1214 (s), 1172 (s), 1154 (m), 1101 (w), 1030 (w), 979 (m), 874 (m), 846 (s), 818 (w), 798 (m), 744 (w), 724 (m), 663 (w), 586 (w), 562 (w), 515 (w). UV-Vis: 386 nm (ε = 65 984), 406 nm (ε = 65 378). quantum yield: Φ = 0.74 ± 0.10.

### 16.5.2. Formatted List

Output with these options: <optionen>: format=\bfseries,delta=(ppm),list=true,use-equal

yield: 17 mg yellow needles (0.04 mmol, 13 %).

mp. = 277 °C (DSC).

<sup>1</sup>H-NMR (600 MHz, CDCl<sub>3</sub>): δ (ppm) = 2.01 (s, 24 H, H-5), 2.31 (s, 12 H, H-1), 6.72–6.74 (m, 2 H, H-11), 6.82 (s, 8 H, H-3), 7.05–7.07 (m, 2 H, H-12), 7.39–7.41 (m, 4 H, H-9), 7.48–7.49 (m, 4 H, H-8).

<sup>13</sup>C-NMR (150 MHz, CDCl<sub>3</sub>): δ (ppm) = 21.2 (+, 4 C, C-1), 23.4 (+, 8 C, C-5), 126.0 (+, 4 C, C-9), 128.2 (+, 8 C, C-3), 130.8 (+, 2 C, C-12), 133.6 (+, 2 C, C-11), 137.0 (+, 4 C, C-8), 138.6 (q, 4 C, C-2), 140.6 (q, 2 C, C-10), 140.8 (q, 8 C, C-4), 141.8 (q, 4 C, C-6), 145.6 (q, 2 C, C-7).

MS (DCP, EI, 60 eV) = 703 (2, M<sup>+</sup>), 582 (1), 462 (1), 249 (13), 120 (41), 105 (100).

MS (MeOH + H<sub>2</sub>O + KI, ESI, 10 eV) = 720 (100, M<sup>+</sup> + OH<sup>-</sup>), 368 (M<sup>+</sup> + 2 OH<sup>-</sup>).

IR (KBr) = 3443 (w), 3061 (w), 2957 (m), 2918 (m), 2856 (w), 2729 (w), 1725 (w), 1606 (s), 1592 (s), 1545 (w), 1446 (m), 1421 (m), 1402 (m), 1357 (w), 1278 (w), 1238 (s), 1214 (s), 1172 (s), 1154 (m), 1101 (w), 1030 (w), 979 (m), 874 (m), 846 (s), 818 (w), 798 (m), 744 (w), 724 (m), 663 (w), 586 (w), 562 (w), 515 (w).

UV-Vis: 386 nm ( $\epsilon = 65\,984$ ), 406 nm ( $\epsilon = 65\,378$ ).

quantum yield:  $\Phi = 0.74 \pm 0.10$ .

### 16.5.3. Crazy

Output for these options: <optionen>:

```

1  format=\color{red}\itshape,
2  list=true,
3  delta=\textcolor{green}{\ch{M+ + H2O}},
4  pos-number=side,
5  coupling-unit=\mega\gram\per\square\second,
6  list-setup=,
7  use-equal

```

*yield*: 17 mg yellow needles (0.04 mmol, 13 %).

*mp.* = 277 °C (DSC).

*<sup>1</sup>H-NMR (600 MHz, CDCl<sub>3</sub>)*:  $\delta$   $M^+ + H_2O$  = 2.01 (s, 24 H, H-5), 2.31 (s, 12 H, H-1), 6.72–6.74 (m, 2 H, H-11), 6.82 (s, 8 H, H-3), 7.05–7.07 (m, 2 H, H-12), 7.39–7.41 (m, 4 H, H-9), 7.48–7.49 (m, 4 H, H-8).

*<sup>13</sup>C-NMR (150 MHz, CDCl<sub>3</sub>)*:  $\delta$   $M^+ + H_2O$  = 21.2 (+, 4 C, C-1), 23.4 (+, 8 C, C-5), 126.0 (+, 4 C, C-9), 128.2 (+, 8 C, C-3), 130.8 (+, 2 C, C-12), 133.6 (+, 2 C, C-11), 137.0 (+, 4 C, C-8), 138.6 (q, 4 C, C-2), 140.6 (q, 2 C, C-10), 140.8 (q, 8 C, C-4), 141.8 (q, 4 C, C-6), 145.6 (q, 2 C, C-7).

*MS (DCP, EI, 60 eV)* = 703 (2,  $M^+$ ), 582 (1), 462 (1), 249 (13), 120 (41), 105 (100).

*MS (MeOH + H<sub>2</sub>O + KI, ESI, 10 eV)* = 720 (100,  $M^+ + OH^-$ ), 368 ( $M^+ + 2 OH^-$ ).

*IR (KBr)* = 3443 (w), 3061 (w), 2957 (m), 2918 (m), 2856 (w), 2729 (w), 1725 (w), 1606 (s), 1592 (s), 1545 (w), 1446 (m), 1421 (m), 1402 (m), 1357 (w), 1278 (w), 1238 (s), 1214 (s), 1172 (s), 1154 (m), 1101 (w), 1030 (w), 979 (m), 874 (m), 846 (s), 818 (w), 798 (m), 744 (w), 724 (m), 663 (w), 586 (w), 562 (w), 515 (w).

UV-Vis: 386 nm ( $\epsilon = 65\,984$ ), 406 nm ( $\epsilon = 65\,378$ ).

*quantum yield*:  $\Phi = 0.74 \pm 0.10$ .

## 17. Commands for mhchem

mhchem isn't loaded automatically any more but only if you've specified `method = mhchem` in the preamble. In the default settings CHEMMACROS uses CHEMFORMULA instead.

CHEMMACROS provides only one command specifically for mhchem.<sup>29</sup> It is meant to place text below of compounds.

► `\mhName[<keyval>]{<formula>}{<text>}`

<sup>29</sup> CHEMFORMULA provides its own possibility.



For example:

```
1 \ce{4 C2H5Cl + Pb / Na -> \mhName{Pb(C2H5)4}{former antiknock additive} + NaCl}
```

$$4 \text{C}_2\text{H}_5\text{Cl} + \text{Pb}/\text{Na} \longrightarrow \text{Pb}(\text{C}_2\text{H}_5)_4 + \text{NaCl}$$

former  
antiknock  
additive

There are several keys to customize `\mhName`.

**mhName** ► **align** = <alignment command> → the alignment of the text in the box it is placed in, default = `\centering`

**mhName** ► **format** = <anything> → the format of the text

**mhName** ► **fontsize** = <font size command> → the fontsize of the text, default = `\tiny`

**mhName** ► **width** = <dim>|auto → the width of the box the text is placed in, default = auto

```
1 \ce{4 C2H5Cl + Pb / Na -> \mhName[fontsize=\footnotesize]{Pb(C2H5)4}{former antiknock additive} + NaCl}\
2 \chemsetup[mhName]{align=\raggedright,fontsize=\small,format=\bfseries\color{red},width=3cm}
3 \ce{4 C2H5Cl + Pb / Na -> \mhName{Pb(C2H5)4}{former antiknock additive} + NaCl}
```

$$4 \text{C}_2\text{H}_5\text{Cl} + \text{Pb}/\text{Na} \longrightarrow \text{Pb}(\text{C}_2\text{H}_5)_4 + \text{NaCl}$$

former  
antiknock  
additive

$$4 \text{C}_2\text{H}_5\text{Cl} + \text{Pb}/\text{Na} \longrightarrow \text{Pb}(\text{C}_2\text{H}_5)_4 + \text{NaCl}$$

**former**  
**antiknock**  
**additive**

## 18. Reaction Environments

### 18.1. Defined by CHEMMACROS

You can use these environments for numbered...

- `\begin{reaction} <formula or mhchem code> \end{reaction}`
- `\begin{reactions} <formula or mhchem code> \end{reactions}`

...and their starred versions for unnumbered reactions.

- `\begin{reaction*} <formula or mhchem code> \end{reaction*}`
- `\begin{reactions*} <formula or mhchem code> \end{reactions*}`

With them you can create (un)numbered reaction equations similar to mathematical equations.

These environments use the `equation/equation*` environments or the `align/align*` environments, respectively, to display the reactions.

<pre> 1 Reaction with counter: 2 \begin{reaction} 3   A -&gt; B 4 \end{reaction} </pre>	<p>Reaction with counter:</p> $A \rightarrow B \quad \{1\}$
---	---

<pre> 1 Reaction without counter: 2 \begin{reaction*} 3   C -&gt; D 4 \end{reaction*} </pre>	<p>Reaction without counter:</p> $C \rightarrow D$
--	--

<pre> 1 Several aligned reactions with counter: 2 \begin{reactions} 3   A &amp;-&gt; B + C \\ 4   D + E &amp;-&gt; F 5 \end{reactions} </pre>	<p>Several aligned reactions with counter:</p> $\begin{array}{lcl} A & \rightarrow & B + C \\ D + E & \rightarrow & F \end{array} \quad \begin{array}{l} \{2\} \\ \{3\} \end{array}$
---	--

<pre> 1 Several aligned reactions without counter: 2 \begin{reactions*} 3   G &amp;-&gt; H + I \\ 4   J + K &amp;-&gt; L 5 \end{reactions*} </pre>	<p>Several aligned reactions without counter:</p> $\begin{array}{lcl} G & \rightarrow & H + I \\ J + K & \rightarrow & L \end{array}$
--	---

If you want to change the layout of the counter tags, you can use

`\renewtagform{<tagname>}[<format>]{<right delim>}{<left delim>}`.<sup>30</sup>

<pre> 1 \renewtagform{reaction}[R \textbf{}]{[]{}]} 2 \begin{reaction} 3   H2O + CO2 &lt;=&gt; H2CO3 4 \end{reaction} </pre>	$H_2O + CO_2 \rightleftharpoons H_2CO_3 \quad [R \ 4]$
--	--

With version 3.3 referencing and the use of  $\mathcal{M}$ Smath's `\intertext` also function properly:

```

1 \begin{reactions}
2   A + 2 B &-> 3 C + D \label{rxn:test}
3   \intertext{Some text in between aligned reactions}
4   3 E + F &<=> G + 1/2 H
5 \end{reactions}
6 See reaction~\ref{rxn:test}.

```

<sup>30</sup> Provided by the mathtools package



Some text in between aligned reactions



See reaction 5.

In the standard setting, i.e. using `method = chemformula` you should not use `\mch` and its relatives inside the reaction environments. They will very likely mess with spacing. In the standard setting charges inside the environments automatically recognize the setting of the option `circled` so there's also no need for the charge commands.

## 18.2. Own Reactions

You can create new types of reactions with the command:

► `\DeclareChemReaction[<keyval>]{<name>}{<math name>}`

`<name>` will be the name of the new environment. `<math name>` is the used math environment. The command has two options.

~~none~~ ► `star = true|false`

~~none~~ ► `arg = true|false`

There is `star`, which will also define a starred version of the new environment, if the starred math environment exists. If it doesn't exist, this will cause an error.

Then there is `arg`, which is used to define an environment with a mandatory argument. Of course this only works, if the used math environment has a mandatory argument.

The predefined environments are defined via

► `\DeclareChemReaction[star]{reaction}{equation}` and

► `\DeclareChemReaction[star]{reactions}{align}`.

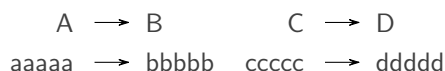
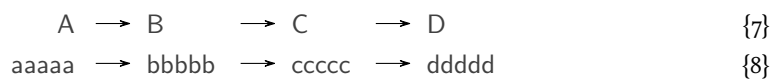
Let's suppose, you'd like to have the alignment behaviour of the `alignat` environment for `CHEM-FORMULA/mhchem` reactions. You could do the following:

`\DeclareChemReaction[star,arg]{reactionsat}{alignat}`

With this the `reactionsat` environment is defined.

```

1 \DeclareChemReaction[star,arg]{reactionsat}{alignat}
2 \begin{reactionsat}{3}
3   A    &-> B    &&-> C    &&-> D \\\
4   aaaaa &-> bbbbb &&-> ccccc &&-> ddddd
5 \end{reactionsat}
6 \begin{reactionsat*}{2}
7   A    &-> B    & C            &-> D \\\
8   aaaaa &-> bbbbb &\quad{} & ccccc &-> ddddd
9 \end{reactionsat*}
```



### 18.3. List of Reactions

CHEMMACROS also provides a command to display a list of the reactions created with the reaction environment.

► \listofreactions

<pre>1 \listofreactions</pre>	
<h2 style="margin: 0;">List of reactions</h2>	
Reaction {1} . . . . .	34
Reaction {2} . . . . .	34
Reaction {3} . . . . .	34
Reaction [R 4] . . . . .	34
Reaction {5} . . . . .	35
Reaction {6} . . . . .	35
Reaction {7} . . . . .	36
Reaction {8} . . . . .	36
Reaction {9}: Autoprotolyse . . . . .	37
Reaction {10}: first step of chain . . . . .	37
Reaction {11}: second step of chain . . . . .	37
Reaction {12}: Synthese von Alkanen . . . . .	61

The Output of this list can be modified by two options:

**reaction** ► **list-name** = <name of the list> → Let's you set the name of the list manually. Default = List of reactions

**reaction** ► **list-entry** = <prefix to each entry> → Let's you set a prefix to each list entry. Default = Reaction

**option** Both default option values recognize the package option **german**.

Instead of using the option **list-name** you also could redefine **\reactionlistname**.

The list lists all reactions with a number and disregards reactions without number. All reaction environments without star have an optional argument which let's you add a description (or caption) for the entry in the list.

```

1 \begin{reaction}[Autoprotolyse]
2   2 H2O <=> H3O+ + OH-
3 \end{reaction}

```

$$2 \text{H}_2\text{O} \rightleftharpoons \text{H}_3\text{O}^+ + \text{OH}^- \quad \{9\}$$

If you use the reactions environment this will not work, though. In this case you can use

► `\AddRxnDesc{<description>}`

```

1 \begin{reactions}
2   Cl "\Lewis{0.,\vphantom{Cl}}" + CH4    &-> HCl + "\Lewis{4.,\vphantom{CH}}" CH3
   \AddRxnDesc{first~step~of~chain} \
3   "\Lewis{4.,\vphantom{CH}}" CH3 + Cl2 &-> CH3Cl + Cl "\Lewis{0.,\vphantom{Cl}}"
   \AddRxnDesc{second~step~of~chain}
4 \end{reactions}

```

$$\text{Cl}\cdot + \text{CH}_4 \rightarrow \text{HCl} + \cdot\text{CH}_3 \quad \{10\}$$

$$\cdot\text{CH}_3 + \text{Cl}_2 \rightarrow \text{CH}_3\text{Cl} + \text{Cl}\cdot \quad \{11\}$$

Note: you don't have to use the phantom commands if you haven't changed the format of the atoms, see section 30 on page 58.

## 19. Phases

### 19.1. Basics

These commands are intended to indicate the phase of a compound.

► `\sld` → (s)

► `\lqd` → (l)

► `\gas` → (g)

► `\aq` → (aq)

The default behaviour of the phases commands has changed to be consistent with IUPAC recommendations. Both `\sld` and `\lqd` have lost their optional argument.

```

1 \ch{C\sld} + 2 H2O\lqd -> CO2\gas + 2 H2\gas\\
2 To make it complete: NaCl\aq.

```

$$\text{C(s)} + 2 \text{H}_2\text{O(l)} \rightarrow \text{CO}_2\text{(g)} + 2 \text{H}_2\text{(g)}$$

To make it complete: NaCl(aq).

With the package option `language = german` (see section 4) you get the german versions.

The IUPAC recommendation to indicate the state of aggregation is to put it in parentheses after the compound [Coh+08]. However, you might want to put it as a subscript which is also very common.

## 20. Newman Projections

The [...] symbols are used to represent the states of aggregation of chemical species. The letters are appended to the formula in parentheses and should be printed in Roman (upright) type without a full stop (period).  
*IUPAC Green Book [Coh+08, p. 54]*

There are two options to customize the output:

**phases** ► **pos** = side|sub → Switch the position of the phase indicator. Default = side

**phases** ► **space** = <dim> → Change the default spacing between compound a phase indicator if **pos** = side.  
A  $\text{T}_{\text{E}}\text{X}$  dimension. Default = .1333em

```
1 \chemsetup[phases]{pos=sub}
2 \ch{C\sld{}} + 2 H2O\lqd{} -> CO2\gas{} + 2 H2\gas{}\
3 To make it complete: NaCl\aq.

C(s) + 2 H2O(l) → CO2(g) + 2 H2(g)
To make it complete: NaCl(aq).
```

### 19.2. Define Own Phases

Depending on the subject of your document you might need to indicate other states of aggregation. You can easily define them.

- `\DeclareChemPhase{<cmd>}[<german>]{<english>}`
- `\RenewChemPhase{<cmd>}[<german>]{<english>}`
- `\phase{<phase>}` → If you need a phase indicator just once or twice.

`\DeclareChemPhase` only defines a phase if <cmd> is not already used by any other command. If it is already used `CHEMMACROS` will either give a warning or an error, depending on the option **strict**. `\RenewChemPhase` only defines a phase if <cmd> is already used and issues a warning/error otherwise.

```
1 \DeclareChemPhase{\aqi}{aq,$\infty$}% aqueous solution at infinite dilution
2 \DeclareChemPhase{\cd}{cd}% condensed phase
3 \RenewChemPhase{\lqd}{lc}% liquid crystal
4 NaOH\aqi\ \ch{H2O\cd} U\phase{cr} A\lqd \
5 \chemsetup[phases]{pos=sub}
6 NaOH\aqi\ \ch{H2O\cd} U\phase{cr} A\lqd

NaOH(aq, $\infty$ ) H2O (cd) U(cr) A(lc)
NaOH(aq, $\infty$ ) H2O(cd) U(cr) A(lc)
```

## 20. Newman Projections

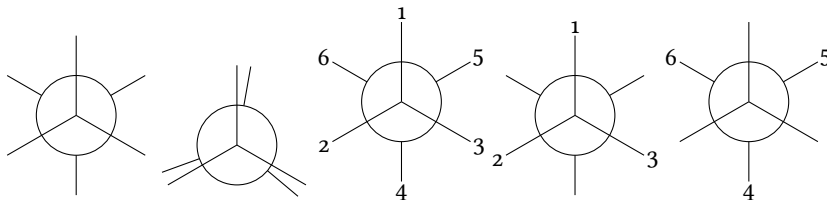
`CHEMMACROS` provides the command

- `\newman[<keyval>](<angle>){<1>,<2>,<3>,<4>,<5>,<6>}`

## 20. Newman Projections

which allows you to create newman projections (uses **TikZ**). With `<angle>` the back atoms are rotated counter clockwise with respect to the front atoms.

```
1 \newman{} \newman(170){}  
2 \newman{1,2,3,4,5,6} \newman{1,2,3} \newman{,,4,5,6}
```



Several options allow customization:

**newman** ► **angle** = `<angle>` → default angle

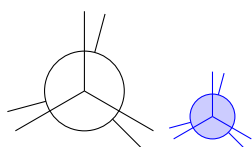
**newman** ► **scale** = `<factor>` → scale the whole projection

**newman** ► **ring** = `<tikz>` → customize the ring with **TikZ** keys

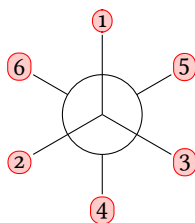
**newman** ► **atoms** = `<tikz>` → customize the nodes within which the atoms are set

**newman** ► **back-atoms** = `<tikz>` → explicitly customize the back atoms

```
1 \chemsetup[newman]{angle=45} \newman{}  
2 \newman[scale=.75,ring={draw=blue,fill=blue!20}]{}
```



```
1 \chemsetup[newman]{atoms={draw=red,fill=red!20,inner sep=2pt,rounded corners}}  
2 \newman{1,2,3,4,5,6}
```



```
1 \chemsetup[newman]{  
2   atoms = {draw=red,fill=red!20,inner sep=2pt,rounded corners},  
3   back-atoms = {draw=blue,fill=blue!20,inner sep=2pt,rounded corners}  
4 }  
5 \newman{1,2,3,4,5,6} \newman(170){1,2,3,4,5,6}
```



## 21. s, p, and Hybrid Orbitals

CHEMMACROS provides the following command to create orbitals:

► `\orbital[<keyval>]{<type>}`

There are the following types available for <type>:

s

p

sp

sp<sup>2</sup>

sp<sup>3</sup>

```
1 \orbital{s} \orbital{p} \orbital{sp} \orbital{sp2} \orbital{sp3}
```



Depending on the type you have different options to modify the orbitals:

`orbital` ► `phase = +/-` → changes the phase of the orbital (all types)

`orbital` ► `scale = <factor>` → changes the size of the orbital (all types)

`orbital` ► `color = <color>` → changes the color of the orbital (all types)

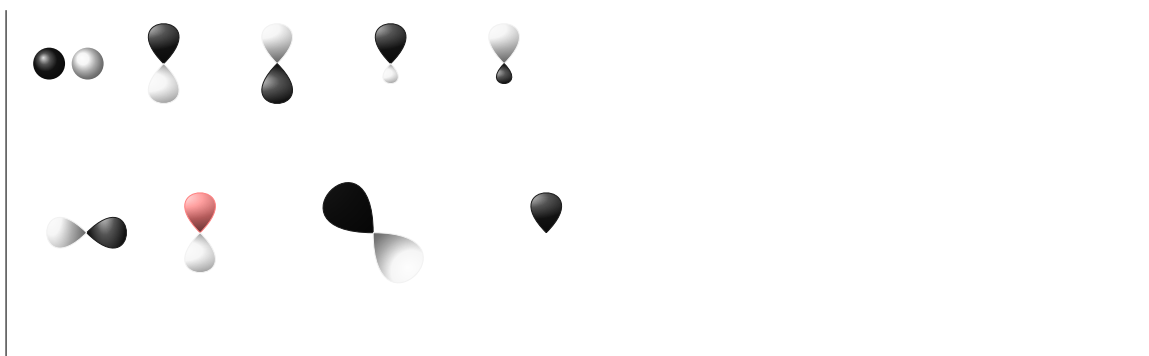
`orbital` ► `angle = <angle>` → rotates the orbitals with a p contribution counter clockwise (all types except s)

`orbital` ► `half = true|false` → displays only half an orbital (only p)

```
1 \orbital{s} \orbital[phase=-]{s}
2 \orbital{p} \orbital[phase=-]{p}
3 \orbital{sp3} \orbital[phase=-]{sp3}
4
5 \orbital[angle=0]{p} \orbital[color=red!50]{p} \orbital[angle=135,scale=1.5]{p}
  \orbital[half]{p}
```



## 21. s, p, and Hybrid Orbitals



Additionally there are two options, with which the `TikZ` behaviour can be changed.

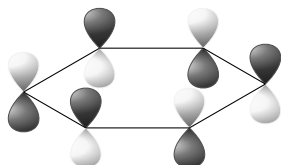
`orbital` ► `overlay` = `true|false` → the orbital “doesn’t need space”; it is displayed with the `TikZ` option `overlay`.

`orbital` ► `opacity` = `<num>` → the orbital becomes transparent; `<value>` can have values between 1 (fully opaque) to 0 (invisible).

```

1 \hspace{1cm}
2 \chemsetup[orbital]{
3   overlay,
4   p/color = black!70
5 }
6 \setbondoffset{0pt}
7 \chemfig{?\orbital{p}-[,1.3]{\orbital[phase=-]{p}}-[:30,1.1]\orbital{p}
8   }-[:150,.9]{\orbital[phase=-]{p}}-[4,1.3]\orbital{p}-[: -150,1.1]{\orbital[phase
   =-]{p}}??}
9 \vspace{7mm}

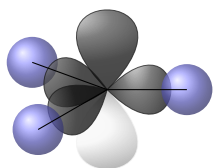
```



```

1 \hspace{2cm}
2 \setbondoffset{0pt}
3 \chemsetup[orbital]{
4   overlay ,
5   opacity = .75 ,
6   p/scale = 1.6 ,
7   s/color = blue!50 ,
8   s/scale = 1.6
9 }
10 \chemfig{\orbital{s}-[: -20]{\orbital[scale=2]{p}}{\orbital[half,angle=0]{p}}{\orbital[half,angle=170]{p}}{\orbital[half,angle=-150]{p}}(-[: -150]\orbital{s})
11 \vspace{1cm}

```



## Part III.

# chemformula

### 22. Setup

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

```

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

```

### 23. 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:

1	<code>\ch{H2O} \\\</code>	$\text{H}_2\text{O}$
2	<code>\ch{Sb2O3} \\\</code>	$\text{Sb}_2\text{O}_3$
3	<code>\ch{H+} \\\</code>	$\text{H}^+$
4	<code>\ch{CrO4^2-} \\\</code>	$\text{CrO}_4^{2-}$
5	<code>\ch{AgCl2} \\\</code>	$\text{AgCl}_2^-$
6	<code>\ch{[AgCl2]-} \\\</code>	$[\text{AgCl}_2]^-$
7	<code>\ch{Y^{99+}} \\\</code>	$\text{Y}^{99+}$
8	<code>\ch{Y^{99+}} \\\</code>	$\text{Y}^{99+}$
9	<code>\ch{H2_{(aq)}} \\\</code>	$\text{H}_{2(\text{aq})}$
10	<code>\ch{NO3-} \\\</code>	$\text{NO}_3^-$
11	<code>\ch{(NH4)2S} \\\</code>	$(\text{NH}_4)_2\text{S}$
12	<code>\ch{^{227}_{90}Th+} \\\</code>	$^{227}_{90}\text{Th}^+$
13	<code>\$V_{\ch{H2O}}\$ \\\</code>	$V_{\text{H}_2\text{O}}$
14	<code>\ch{Ce^{IV}} \\\</code>	$\text{Ce}^{\text{IV}}$
15	<code>\ch{KCr(SO4)2 * 12 H2O}</code>	$\text{KCr}(\text{SO}_4)_2 \cdot 12 \text{H}_2\text{O}$

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:

1	<code>\ch{A + B -&gt;[a] C} \\\</code>	$A + B \xrightarrow{a} C$
2	<code>\ce{A + B -&gt;[a] C}</code>	$A + B \xrightarrow{a} C$

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

1	<code>\ch{2H2O} \\\</code>	$2\text{H}_2\text{O}$
2	<code>\ch{2 H2O}</code>	$2 \text{H}_2\text{O}$

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**.

► `\chemsetup[chemformula]{<options>}`

## 24. Stoichiometric Factors

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

## 24. Stoichiometric Factors

1	<code>\ch{2} \</code>	
2	<code>\ch{12}</code>	
3		2
4	% decimals:	12
5	<code>\ch{3.5} \</code>	3.5
6	<code>\ch{5,75}</code>	5.75
7		$\frac{3}{2}$
8	% fractions:	$1\frac{1}{2}$
9	<code>\ch{3/2} \</code>	
10	<code>\ch{1_1/2}</code>	

You have to be a little bit careful with the right syntax but I believe it is rather intuitive.

```
1 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. What's inside the parenthesis is typeset as is.

1	<code>\ch{(1/2) H2O} \ch{1/2 H2O} \ch{0.5 H2O}</code>	$(1/2)\text{H}_2\text{O}$ $\frac{1}{2}\text{H}_2\text{O}$ $0.5\text{H}_2\text{O}$
---	---	---

You can find many examples like the following for stoichiometric factors in parentheses in the IUPAC Green Book [Coh+o8]:



There are a few possibilities to customize the output.

- **decimal-marker** = <marker> → the symbol to indicate the decimal. Default = .
- **frac-style** = math|xfrac|nicefrac → determines how fractions are displayed. Default = math
- **stoich-space** = <dim> → The space that is placed after the stoichiometric factor. Default = .1667em

1	<code>\ch[decimal-marker={,}]{3.5} \ch[decimal-marker={\cldot\$}]{3,5}</code>
	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.

1	<code>\ch[frac-style=xfrac]{3/2} \ch[frac-style=xfrac]{1_1/2}</code>
	$\frac{3}{2}$ $1\frac{1}{2}$

**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:

```

1 \DeclareInstance{xfrac}{chemformula-text-frac}{text}
2 {
3   slash-left-kern = -.15em ,
4   slash-right-kern = -.15em
5 }

```

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

```

1 \DeclareInstance{xfrac}{chemformula-text-frac}{text}
2 {
3   scale-factor      = 1 ,
4   denominator-bot-sep = -.2ex ,
5   denominator-format = \scriptsize #1 ,
6   numerator-top-sep = -.2ex ,
7   numerator-format = \scriptsize #1
8 }

```

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

```

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

```

$\frac{3}{2}$   $1\frac{1}{2}$

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

```

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

```

$2 \text{H}_2\text{O}$   $2 \text{H}_2\text{O}$

## 25. 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.

```

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

```

$\text{H}_2\text{SO}_4$   $[\text{Cu}(\text{NH}_3)_4]^{2+}$

### 25.1. Adducts

**CHEMFORMULA** has two identifiers which will create adducts.

► `\ch{A.B}` →

► `\ch{A*B}` →

## 25. Compounds

1	<code>\ch{CaSO4.H2O} \\</code>	$\text{CaSO}_4 \cdot \text{H}_2\text{O}$
2	<code>\ch{CaSO4*H2O}</code>	$\text{CaSO}_4 \cdot \text{H}_2\text{O}$

Since numbers in a compound always are treated as subscripts (see section 25.2) you sometimes need to introduce stoichiometric factors for the right output:

1	<code>\ch{Na3PO4*12H2O} \\</code>	$\text{Na}_3\text{PO}_4 \cdot {}_{12}\text{H}_2\text{O}$
2	<code>\ch{Na3PO4* 12 H2O} \\</code>	$\text{Na}_3\text{PO}_4 \cdot 12 \text{H}_2\text{O}$
3	<code>\ch{Na3PO4 * 12 H2O}</code>	$\text{Na}_3\text{PO}_4 \cdot 12 \text{H}_2\text{O}$

### 25.2. Subscripts

All numbers in a compound are treated as subscripts.

1	<code>\ch{H2SO4}</code>	$\text{H}_2\text{SO}_4$
---	-------------------------	-------------------------

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

1	<code>\ch{A_nB_m}</code>	$A_nB_m$
---	--------------------------	----------

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

1	<code>\ch{A_{n\$}B_{m\$}} \\</code>	$A_nB_m$
2	<code>\ch{NaCl_{(aq)}}</code>	$\text{NaCl}_{(\text{aq})}$

### 25.3. Commands

Commands are allowed in a compound:

1	<code>\ch{\textbf{A2}B3} \ch{A2\color{red}B3}</code>	$A_2B_3 \quad A_2B_3$
---	--	-----------------------

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.

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

See section 27.1 for a way around this.

### 25.4. 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 25.5.

1	<code>\ch{A+B} \ch{AB+} \</code>	$A \equiv B \text{ AB}^+$
2	<code>\ch{A-B} \ch{AB-}</code>	$A - B \text{ AB}^-$

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.

1	<code>\ch{A^{x-}} \</code>	$A^{x-}$
2	<code>\ch{A^x-} \</code>	$A^{x-}$
3	<code>\ch{A^{x}-} \</code>	$A^{x-}$
4	<code>\ch{A^{x-}} \</code>	$A^{x-}$
5	<code>\ch{RNO2^{-.}} \</code>	$\text{RNO}_2^{\cdot-}$
6	<code>\ch{^31H} \</code>	$^3_1\text{H}$
7	<code>\ch{^{14}6C} \</code>	$^{14}_6\text{C}$
8	<code>\ch{^{58}_{26}Fe} \</code>	$^{58}_{26}\text{Fe}$
9	<code>\ch{NO^*}</code>	$\text{NO}^*$

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

1	<code>\ch{SO4^{2-}} \ch{Ca^{2+} SO4^{2-}}</code>	$\text{SO}_4^{2-} \text{ Ca}^{2+} \text{SO}_4^{2-}$
---	--	---

**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`.

1	<code>\chemsetup[option]{circled=all}</code>	$\text{H}^{\oplus} + \text{OH}^{\ominus} \rightleftharpoons \text{H}_2\text{O}$
2	<code>\ch{H+ + OH- &lt;=&gt; H2O}</code>	

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

1	<code>\ch{^33B} \ch{{}^33B} \ch{3^3B} \ch{B^3} \ch{B3^3} \</code>	
2	<code>\ch{^{23}_{123}B} \ch{{}^{23}_{123}B} \ch{{}_{123}^{23}B} \ch{B^{23}} \ch{B_{123}^{23}} \</code>	
3	<code>\ch{^{123}_{23}B} \ch{{}^{123}_{23}B} \ch{{}_{23}^{123}B} \ch{B^{123}} \ch{B_{23}^{123}}</code>	

$^3\text{B}$   $^3_3\text{B}$   $^3_3\text{B}$   $\text{B}^3$   $\text{B}_3^3$   
 $^{23}_{123}\text{B}$   $^{23}_{123}\text{B}$   $^{23}_{123}\text{B}$   $\text{B}^{23}$   $\text{B}_{123}^{23}$   
 $^{123}_{23}\text{B}$   $^{123}_{23}\text{B}$   $^{123}_{23}\text{B}$   $\text{B}^{123}$   $\text{B}_{23}^{123}$

- 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 50f.

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:  $\text{SO}_4^{2-}$ ,  $(\text{SO}_4)^{2-}$ . The staggered arrangement is now recommended. *IUPAC Green Book [Coh+08, p. 51]*

## 25.5. Bonds

### 25.5.1. Native Bonds

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

1	single: <code>\ch{CH3-CH3} \</code>	single: $\text{CH}_3\text{--CH}_3$
2	double: <code>\ch{CH2=CH2} \</code>	double: $\text{CH}_2=\text{CH}_2$
3	triple: <code>\ch{CH\equiv CH}</code>	triple: $\text{CH}\equiv\text{CH}$

### 25.5.2. 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 3.

Table 3: Bonds available with `\bond`.

name	appearance	aliases
single	—	normal, sb
double	=	db
triple	≡	tp
dotted	⋯	semisingle
deloc	⋮	semidouble
tdeloc	≡	semitriple
co>	→	coordright
<co	←	coordleft

1	<code>\ch{C\bond{sb}C\bond{db}C\bond{tp}C\bond{deloc}C\bond{tdeloc}C\bond{co&gt;}C\bond{&lt;co}C}</code>
	$\text{C}-\text{C}=\text{C}\equiv\text{C}\cdots\text{C}\equiv\text{C}\rightarrow\text{C}\leftarrow\text{C}$



**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:

```

1 \DeclareChemBond{single}
2   { \draw[chembond] (chemformula-bond-start) -- (chemformula-bond-end) ; }
3 \DeclareChemBond{coordright}
4   { \draw[chembond,butt cap->] (chemformula-bond-start) -- (chemformula-bond
   -end) ; }
5 \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 $\mathbf{k}$ Z** style of the bonds `chembond`.

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

```

1 \usetikzlibrary{decorations.pathreplacing}
2 \makeatletter
3 \DeclareChemBond{dashed}
4   {
5     \draw[
6       chembond,
7       decorate,
8       decoration={ticks,segment length=\chemformula@bondlength/10,amplitude=1.5
9       pt}]
10      (chemformula-bond-start) -- (chemformula-bond-end) ;
11   }
12 \makeatother
13 \chemsetup[chemformula]{bond-length=2ex}
14 \ch{C\bond{dashed}C}

```

C $\text{---}$ 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.

## 25.6. Customization

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

- ▶ `subscript-vshift` = <dim> → Extra vertical shift of the subscripts. Default = 0pt
- ▶ `subscript-style` = text|math → Style that is used to typeset the subscripts. Default = text

- **charge-hshift** = <dim> → Shift of superscripts when following a subscript. Default = .5ex
- **charge-vshift** = <dim> → Extra vertical shift of the superscripts. Default = 0pt
- **charge-style** = text|math → Style that is used to typeset the superscripts. Default = text
- **adduct-space** = <dim> → Space to the left and the right of the adduct point. Default = .1333em
- **bond-length** = <dim> → The length of the bonds. Default = 1.1667ex
- **bond-offset** = <dim> → Space between bond and atoms. Default = .07em
- **bond-style** = <tikz> → TikZ options for the bonds. Initially empty.
- **radical-style** = <tikz> → TikZ options for the radical point. Initially empty.
- **radical-radius** = <dim> → The radius of the radical point. Default = .2ex

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

1	<code>\ch{SO4^2-} \ch{NH4+} \ch{Na+}</code>	$\text{SO}_4^{2-} \text{NH}_4^+ \text{Na}^+$
---	---	--

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**.

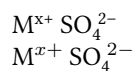
1	<code>\ch{SO4^2-} \ch{NH4+} \ch{Na+} \\\</code>	$\text{SO}_4^{2-} \text{NH}_4^+ \text{Na}^+$
2	<code>\chemsetup[chemformula]{charge-hshift=.5ex}</code>	$\text{SO}_4^{2-} \text{NH}_4^+ \text{Na}^+$
3	<code>\ch{SO4^2-} \ch{NH4+} \ch{Na+} \\\</code>	$\text{SO}_4^{2-} \text{NH}_4^+ \text{Na}^+$
4	<code>\chemsetup[chemformula]{charge-hshift=.5pt}</code>	$\text{SO}_4^{2-} \text{NH}_4^+ \text{Na}^+$
5	<code>\ch{SO4^2-} \ch{NH4+} \ch{Na+}</code>	

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**.

1	<code>\ch[charge-hshift=0pt]{C5H11+} \ch[charge-hshift=0pt]{SO4^2-} \\\</code>	$\text{C}_5\text{H}_{11}^+ \text{SO}_4^{2-}$
2	<code>\ch{C5H11+} \ch{SO4^2-} \\\</code>	$\text{C}_5\text{H}_{11}^+ \text{SO}_4^{2-}$
3	<code>\ch[charge-hshift=1ex]{C5H11+} \ch[charge-hshift=1ex]{SO4^2-} \\\</code>	$\text{C}_5\text{H}_{11}^+ \text{SO}_4^{2-}$
4	<code>\ch[charge-hshift=full]{C5H11+} \ch[charge-hshift=full]{SO4^2-}</code>	$\text{C}_5\text{H}_{11}^+ \text{SO}_4^{2-}$

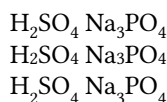
If you don't want the charges to be typeset in text mode you can switch to math mode:

1	<code>\ch{M^x+} \ch{SO4^2-} \\\</code>
2	<code>\chemsetup[chemformula]{charge-style = math}</code>
3	<code>\ch{M^x+} \ch{SO4^2-}</code>



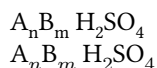
The option `subscript-vshift` can be used to adjust the vertical shift of the subscripts:

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



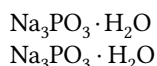
You can choose the mode subscripts are typeset in the same way as it is possible for the charges:

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



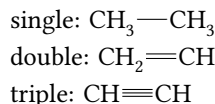
The option `adduct-space` sets the space left and right to the adduct symbol `.`.

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



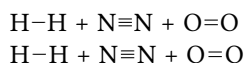
Changing the length of the bonds:

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



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

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



## 26. Special Input Types

There are some “special type” input groups.

### 26.1. Single Token Groups

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

## 26. Special Input Types

- `\ch{ + }` → + creates the plus sign between compounds with space around it:

`\ch{2 Na + Cl2}` 2 Na + Cl<sub>2</sub>

- `\ch{ v }` → ↓ sign for precipitate: `\ch{BaSO4 v}` BaSO<sub>4</sub>↓

- `\ch{ ^ }` → ↑ sign for escaping gas<sup>31</sup>: `\ch{H2 ^}` H<sub>2</sub>↑

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

- `plus-space = <dim>` → Default = .3em

1	<code>\ch{A + B}\</code>	A + B
2	<code>\ch[plus-space=4pt]{A + B}</code>	A + B

### 26.2. Option Input

This is an experimental feature and may well be dropped in future versions.

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.

1	<code>\ch{H2O +}\textcolor{red}{\ch{H2SO4}}\ch{-&gt; H3O+ + HSO4-} \</code>
2	<code>\ch{H2O +}\ch[subscript-vshift=2pt]{H2SO4}\ch{-&gt; H3O+ + HSO4-} \</code>
	$\text{H}_2\text{O} + \textcolor{red}{\text{H}_2\text{SO}_4} \rightarrow \text{H}_3\text{O}^+ + \text{HSO}_4^-$ $\text{H}_2\text{O} + \text{H}_2\text{SO}_4 \rightarrow \text{H}_3\text{O}^+ + \text{HSO}_4^-$

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.

1	<code>\ch{H2O +}\textcolor{red}{\ch{H2SO4}}\ch{-&gt; H3O+ + HSO4-} \</code>
2	<code>\ch{H2O + @\format=\color{red}} H2SO4 -&gt; H3O+ + HSO4-} \</code>
3	or of course:\
4	<code>\ch{H2O + \textcolor{red}{H2SO4} -&gt; H3O+ + HSO4-}\[1em]</code>
5	<code>\ch{H2O +}\ch[subscript-vshift=2pt]{H2SO4}\ch{-&gt; H3O+ + HSO4-} \</code>
6	<code>\ch{H2O + @\subscript-vshift=2pt} H2SO4 -&gt; H3O+ + HSO4-}</code>
	$\text{H}_2\text{O} + \textcolor{red}{\text{H}_2\text{SO}_4} \rightarrow \text{H}_3\text{O}^+ + \text{HSO}_4^-$ $\text{H}_2\text{O} + \textcolor{red}{\text{H}_2\text{SO}_4} \rightarrow \text{H}_3\text{O}^+ + \text{HSO}_4^-$ <p>or of course:</p> $\text{H}_2\text{O} + \textcolor{red}{\text{H}_2\text{SO}_4} \rightarrow \text{H}_3\text{O}^+ + \text{HSO}_4^-$ $\text{H}_2\text{O} + \text{H}_2\text{SO}_4 \rightarrow \text{H}_3\text{O}^+ + \text{HSO}_4^-$ $\text{H}_2\text{O} + \text{H}_2\text{SO}_4 \rightarrow \text{H}_3\text{O}^+ + \text{HSO}_4^-$

<sup>31</sup> Is this the correct English term? Please correct me if it isn't.

## 27. Escaped Input

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

### 27.1. 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>' }`

```

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

II  
CaO  
...Na + ... Cl<sub>2</sub> → ...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.

### 27.2. 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.

► `\ch{ $<escaped math>$ }`

1	escaped text: <code>\ch{"\$x\$" H2O} \</code>	escaped text: $x\text{H}_2\text{O}$
2	escaped math: <code>\ch{"\$x\$ H2O} \</code>	escaped math: $x\text{H}_2\text{O}$
3	<code>\ch{"\$2n\$ Na + \$n\$ Cl2 -&gt; \$2n\$ NaCl}"</code>	$2n\text{Na} + n\text{Cl}_2 \rightarrow 2n\text{NaCl}$

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

► `math-space = <dim> → Default = .1667em`

1	<code>\ch{"\$2n\$ Na + \$n\$ Cl2 -&gt; \$2n\$ NaCl}"</code>	$2n\text{Na} + n\text{Cl}_2 \rightarrow 2n\text{NaCl}$
2	<code>\chemsetup[chemformula]{math-space=.25em}</code>	$2n\text{Na} + n\text{Cl}_2 \rightarrow 2n\text{NaCl}$
3	<code>\ch{"\$2n\$ Na + \$n\$ Cl2 -&gt; \$2n\$ NaCl}"</code>	$A- > B$
4	<code>\ch{"\$A-&gt;B\$}"</code>	

## 28. Arrows

### 28.1. Arrow types

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

- ▶ `\ch{ -> }` → → standard right arrow
- ▶ `\ch{ <- }` → ← standard left arrow
- ▶ `\ch{ -/> }` → ⇏ does not react (right)
- ▶ `\ch{ </- }` → ⇏ does not react (left)
- ▶ `\ch{ <-> }` → ↔ resonance arrow
- ▶ `\ch{ <> }` → ⇌ reaction in both directions
- ▶ `\ch{ == }` → = stoichiometric equation
- ▶ `\ch{ <=> }` → ⇌ equilibrium arrow
- ▶ `\ch{ <=>> }` → ⇌ unbalanced equilibrium arrow to the right
- ▶ `\ch{ <=>< }` → ⇌ unbalanced equilibrium arrow to the left
- ▶ `\ch{ <o> }` → ↔ isolobal arrow

All these arrows are drawn with **Ti $\mathbf{k}$ Z**.

```

1 \ch{H2 + Cl2 -> 2 HCl} \\
2 \ch{H2O + CO3^2- <=> OH- + HCO3-} \\
3 \ch{A <- B} \\
4 \ch{\{[CH2=CH-CH2]- <-> [CH2-CH=CH2]- \}} \\
5 \ch{A <> B} \\
6 \ch{H+ + OH- <=>> H2O} \\
7 \ch{2 NO2 <=>< N2O4}

H2 + Cl2 → 2 HCl
H2O + CO32- ⇌ OH- + HCO3-
A ← B
{[CH2=CH-CH2]- ↔ [CH2-CH=CH2]-}
A ⇌ B
H+ + OH- ⇌ H2O
2 NO2 ⇌ N2O4

```

### 28.2. Labels

The arrows take two optional arguments to label them.

- ▶ `\ch{ ->[<above>][<below>] }`

1	<code>\ch{A -&gt;[a] B} \\</code>	$A \xrightarrow{a} B$
2	<code>\ch{A -&gt;[a][b] B} \\</code>	$A \xrightarrow[b]{a} B$
3	<code>\ch{A -&gt;[\SI{100}{\celsius}] B}</code>	$A \xrightarrow{100\text{ }^{\circ}\text{C}} B$

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

1	<code>\ch{A -&gt;[H2O] B} \\</code>	$A \xrightarrow{\text{H}_2\text{O}} B$
2	<code>\ch{A -&gt;[ H2O ] B} \\</code>	$A \xrightarrow{\text{H}_2\text{O}} B$
3	<code>\ch{A -&gt;[ "\ox{2,Ca}" F2 ] B} \\</code>	$A \xrightarrow[\text{CaF}_2]{\text{II}}$
4	<code>\ch{A -&gt;[\$\Delta\$,~ \[H+ \]] B}</code>	$A \xrightarrow[\Delta, [\text{H}^+]]{} B$

If you leave the blanks `CHEMFORMULA` treats the groups inside the square brackets as separated 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.

1	<code>\ch{A -&gt;[a] B} \\</code>	$A \xrightarrow{a} B$
2	<code>\ch{A -&gt;[ab] B} \\</code>	$A \xrightarrow{ab} B$
3	<code>\ch{A -&gt;[abc] B} \\</code>	$A \xrightarrow{abc} B$
4	<code>\ch{A -&gt;[abc~abc] B} \\</code>	$A \xrightarrow{abc\ abc} B$
5	% needs the ‘chemfig’ package:	
6	<code>\setatomsep{15pt}</code>	
7	<code>\ch{A -&gt;[ "\chemfig{-[:30]-[:30]OH}" ] B} \\</code>	$A \xrightarrow{\text{OH}} B$
8	<code>\ch{A -&gt;[[ ] B} vs. \ch{A -&gt;[\[ \]] B}</code>	$A \xrightarrow{[ ]} B \text{ vs. } A \xrightarrow{[\[ \]]} B$

### 28.3. Customization

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

- **arrow-offset** = <dim> → 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. Default = 1.5ex
- **arrow-yshift** = <dim> → Shifts an arrow up (positive value) or down (negative value). Default = 0pt
- **arrow-ratio** = <factor> → The ratio of the arrow lengths of the unbalanced equilibrium. .4 would mean that the length of the shorter arrow is 0.4× the length of the longer arrow. Default = .6

- **compound-sep** = <dim> → The space between compounds and the arrows. Default = 1ex
- **label-offset** = <dim> → The space between the labels and the arrows. Default = 2pt
- **label-style** = <font command> → The relative font size of the labels. Default = `\footnotesize`

The following code shows the effect of the different options on the  $\rightleftharpoons$  arrow:

```

1  standard: \ch{A <=>>[x][y] B} \\
2  longer: \ch[arrow-offset=12pt]{A <=>>[x][y] B} \\
3  higher: \ch[arrow-yshift=2pt]{A <=>>[x][y] B} \\
4  more balanced: \ch[arrow-ratio=.8]{A <=>>[x][y] B} \\
5  labels further away: \ch[label-offset=4pt]{A <=>>[x][y] B} \\
6  larger distance to compounds: \ch[compound-sep=2ex]{A <=>>[x][y] B} \\
7  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

## 28.4. 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

```

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

```

In order to define arrows yourself you need to know the basics of *TikZ*.<sup>32</sup> 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  $\rightleftharpoons$ .

(cf\_arrow\_mid\_end) The end of the shorter arrow in types like  $\rightleftharpoons$ .

<sup>32</sup> Please see the pgfmanual for details.

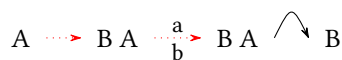


cf, left cf, right cf **CHEMFORMULA**'s own arrow heads.

```

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

```

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

\draw [-cf](cf_arrow_start) (cf_arrow_end);
\draw [->,red] (cf_arrow_start) (cf_arrow_end) ;
A → B

```

## 29. Names

### 29.1. 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:

<pre> 1 \ch{!(ethanol)( CH2CH2OH )} </pre>	$\begin{array}{c} \text{CH}_2\text{CH}_2\text{OH} \\ \text{ethanol} \end{array}$
--	--

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.

```

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

```

### 30. *Format and Font*

H <sub>2</sub> O	H <sub>2</sub> O	H <sub>2</sub> O	H <sub>2</sub> O	H <sub>3</sub> O <sup>+</sup>
water	water	2n - 1	H <sub>2</sub> O	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.

1	<code>\ch{H2O~(!)} \l</code>	H <sub>2</sub> O (!)
2	<code>\ch{A!{}}{() }</code>	A!()

## 29.2. Customization

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

- **name-format** = <commands> → The format of the name. This can be arbitrary input. Default = `\scriptsize\centering`
- **name-width** = <dim>|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. Default = auto

```

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

```

$$\text{H}_2\text{SO}_4 \longrightarrow \text{B}$$

$$\text{H}_2\text{SO}_4 \longrightarrow \text{B}$$

$$\text{H}_2\text{SO}_4 \longrightarrow \text{B}$$

$$\text{N: acid}$$

$$\text{H}_2\text{SO}_4 \longrightarrow \text{B}$$

$$\text{acid}$$

## 30. 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:

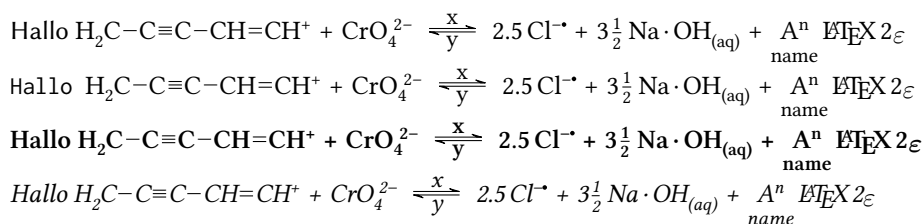
$$\text{H}_2\text{C}-\text{C}\equiv\text{C}-\text{CH}=\text{CH}^+ + \text{CrO}_4^{2-} \xrightleftharpoons[\text{y}]{\text{x}} 2.5 \text{Cl}^\bullet + 3\frac{1}{2} \text{Na}\cdot\text{OH}_{(\text{aq})} + \text{A}^{\text{n}} \quad \text{\LaTeXe}$$

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

```

1 \sffamily Hallo \sample \\
2 \ttfamily Hallo \sample \normalfont \\
3 \bfseries Hallo \sample \normalfont \\
4 \itshape Hallo \sample

```



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

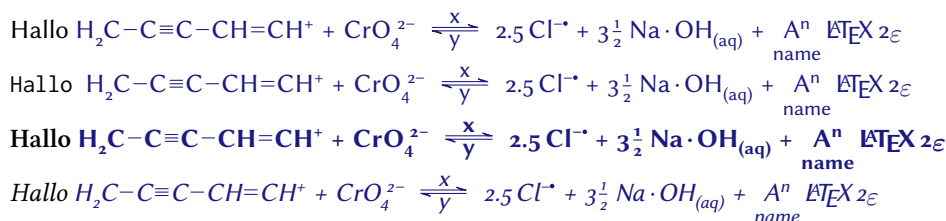
If you want to change the default format you need to use this option:

- **format** = <anything> → Adds arbitrary code before the output of **\ch**.

```

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

```



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

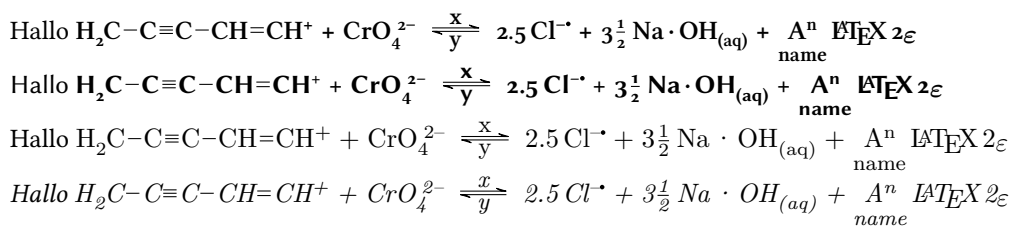
- **font-family** = <family> → Changes the fontfamily of the output with **\fontfamily{<family>}\selectfont**.
- **font-series** = <series> → Changes the fontseries of the output with **\fontseries{<series>}\selectfont**.
- **font-shape** = <shape> → Changes the fontshape of the output with **\fontshape{<shape>}\selectfont**.

```

1 \chemsetup[chemformula]{font-series=bx}
2 Hallo \sample \\
3 \sffamily Hallo \sample \normalfont \\
4 \chemsetup[chemformula]{font-family=lmr,font-series=m} Hallo \sample \normalfont
  \\
5 \itshape Hallo \sample

```

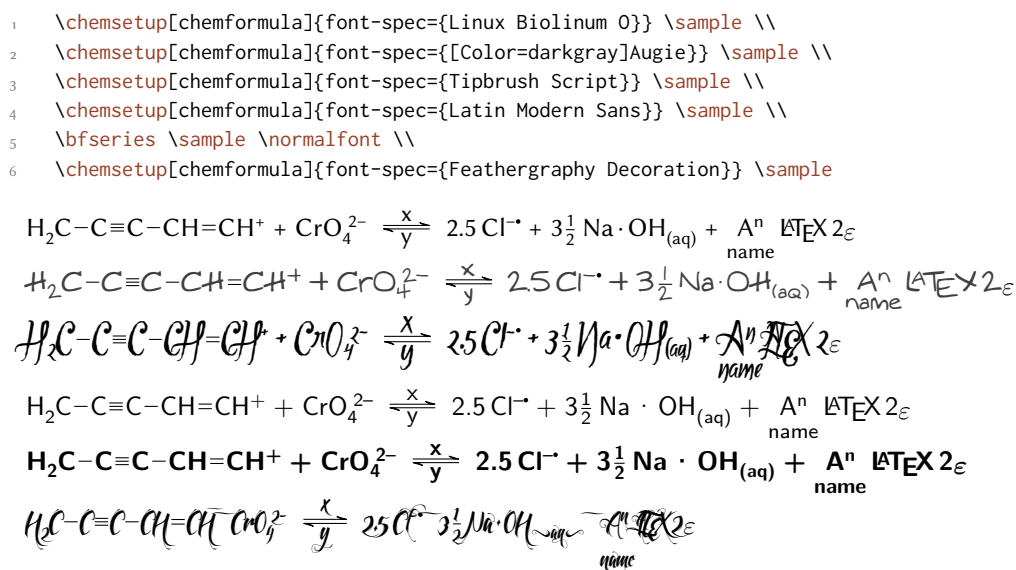
### 31. Usage In Math Equations



If you're using  $\text{X}_{\text{Y}}\text{L}^{\text{A}}\text{T}_{\text{E}}\text{X}$  or  $\text{LuaL}^{\text{A}}\text{T}_{\text{E}}\text{X}$  and have loaded `fontspec`<sup>33</sup> you have the possibility to set the font with it:

► `font-spec` = {<font>} or with options

► `font-spec` = {[<options>]<font>}



### 31. 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`.

<sup>33</sup> CTAN: `fontspec`

## 32. Further Examples

```

1 \begin{align}
2 \quad \text{\ch{H2O}} &\xrightarrow{a} \text{\ch{H2SO4}} & (1) \\
3 \quad \text{\ch{Cl2}} &\xrightarrow{x} \text{\ch{CH4}} & (2)
4 \end{align}
5
6 \begin{align*}
7 \quad \text{\ch{RNO2}} &\xrightleftharpoons{+e^-} \text{\ch{RNO2^{\cdot-}}} \\
8 \quad \text{\ch{RNO2^{\cdot-}}} &\xrightleftharpoons{+e^-} \text{\ch{RNO2^{2-}}}
9 \end{align*}
10
11
12 \end{align*}

```

## 32. Further Examples

This section presents some examples of a possible usage.

```

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

```

$$n \text{ CO} + (2n + 1) \text{ H}_2 \xrightarrow[\text{Synthesegas}]{200^\circ \text{C} [\text{CoNi}]} \text{C}_{n+1}\text{H}_{2n+2} + n \text{ H}_2\text{O} \quad \{12\}$$

```

1 \begin{reactions*}
2 "a)" &\& \text{\ch{CH4}} + \text{\ch{Cl2}} &\&\> \text{\ch{CH3Cl}} + \text{\ch{HCl}} &\&\& "{\small Chlormethan/Methylchlorid}" \\
3 "b)" &\& \text{\ch{CH3Cl}} + \text{\ch{Cl2}} &\&\> \text{\ch{CH2Cl2}} + \text{\ch{HCl}} &\&\& "{\small Dichlormethan/Methylenchlorid}" \\
4 "c)" &\& \text{\ch{CH2Cl2}} + \text{\ch{Cl2}} &\&\> \text{\ch{CHCl3}} + \text{\ch{HCl}} &\&\& "{\small Trichlormethan/Chloroform}" \\
5 "d)" &\& \text{\ch{CHCl3}} + \text{\ch{Cl2}} &\&\> \text{\ch{CCl4}} + \text{\ch{HCl}} &\&\& "{\small Tetrachlormethan/Tetrachlorkohlenstoff}" \\
6 \end{reactions*}

```

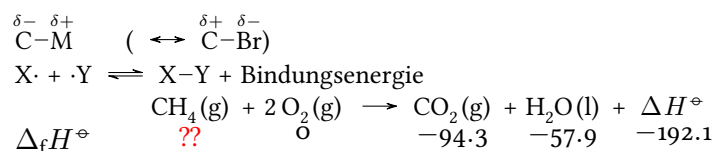
a)	$\text{CH}_4 + \text{Cl}_2 \longrightarrow \text{CH}_3\text{Cl} + \text{HCl}$	Chlormethan/Methylchlorid
b)	$\text{CH}_3\text{Cl} + \text{Cl}_2 \longrightarrow \text{CH}_2\text{Cl}_2 + \text{HCl}$	Dichlormethan/Methylenchlorid
c)	$\text{CH}_2\text{Cl}_2 + \text{Cl}_2 \longrightarrow \text{CHCl}_3 + \text{HCl}$	Trichlormethan/Chloroform
d)	$\text{CHCl}_3 + \text{Cl}_2 \longrightarrow \text{CCl}_4 + \text{HCl}$	Tetrachlormethan/Tetrachlorkohlenstoff

```

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

```

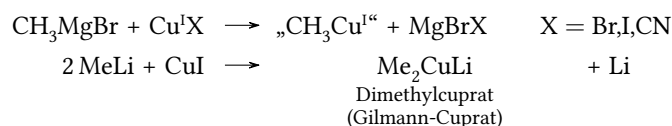
## 32. Further Examples



```

1 \begin{reactions*}
2 CH3MgBr + "\ox{*1,Cu}" X &-> "\glqq" CH3 "\ox{*1,Cu}\grqq" + MgBrX "\quad X
   ~$=-Br,I,CN" \\\
3 2 MeLi + CuI &-> !(Dimethylcuprat~(Gilman-Cuprat))( Me2CuLi ) + Li
4 \end{reactions*}

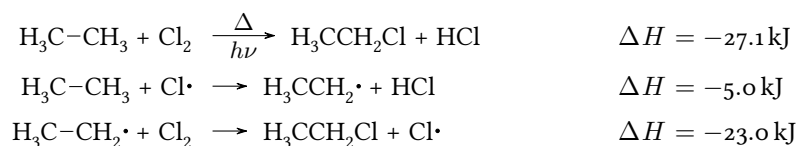
```



```

1 % needs 'chemfig'
2 \begin{reactions*}
3   H3C-CH3 + Cl2 &->[\Delta][h\nu] H3CCH2Cl + HCl
4   & & \&"\Enthalpy{-27.1}" \\
5   H3C-CH3 + "\Lewis{0.,Cl}" &-> H3CCH2 "\Lewis{0.,\vphantom{H}}" +
6   HCl & \&"\Enthalpy{-5.0}" \\
7   H3C-CH2 "\Lewis{0.,\vphantom{H}}" + Cl2 &-> H3CCH2Cl + "\Lewis{0.,Cl}"
8   & \&"\Enthalpy{-23.0}"
9 \end{reactions*}

```

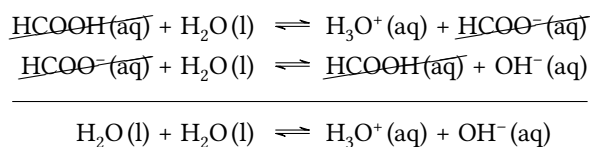


The following example shows how the cancelling of compounds could be done.<sup>34</sup>

```

1 % needs 'cancel'
2 \begin{align*}
3 \quad \text{\textcolor{black}{\cancel{HCOOH}}\text{\textcolor{black}{\aq}}} + \text{\textcolor{black}{H2O}}\text{\textcolor{black}{\lqd}} \quad &\text{\textcolor{black}{\&}}\text{\textcolor{black}{\<}}\text{\textcolor{black}{\>}} \text{\textcolor{black}{H3O}}^+\text{\textcolor{black}{\aq}} + \text{\textcolor{black}{\cancel{HCOO}}}\text{\textcolor{black}{\aq}} \quad \backslash\backslash
4 \quad \text{\textcolor{black}{\cancel{HCOO}}}\text{\textcolor{black}{\aq}} + \text{\textcolor{black}{H2O}}\text{\textcolor{black}{\lqd}} \quad &\text{\textcolor{black}{\&}}\text{\textcolor{black}{\<}}\text{\textcolor{black}{\>}} \text{\textcolor{black}{\cancel{HCOOH}}}\text{\textcolor{black}{\aq}} + \text{\textcolor{black}{OH}}^-\text{\textcolor{black}{\aq}} \quad \backslash[-1ex]
5 \cline{1-2}
6 \quad \text{\textcolor{black}{H2O}}\text{\textcolor{black}{\lqd}} + \text{\textcolor{black}{H2O}}\text{\textcolor{black}{\lqd}} \quad &\text{\textcolor{black}{\&}}\text{\textcolor{black}{\<}}\text{\textcolor{black}{\>}} \text{\textcolor{black}{H3O}}^+\text{\textcolor{black}{\aq}} + \text{\textcolor{black}{OH}}^-\text{\textcolor{black}{\aq}}
7 \end{align*}

```



<sup>34</sup> Inspired by a question on TeX.SE: <http://tex.stackexchange.com/q/30118/5049>

# Part IV.

# ghsystem

## 33. Setup

All of **GHSYSTEM**'s options belong to the module **ghsystem**. This means they can be setup with

```
1 \chemsetup[ghsystem]{<options>} or
2 \chemsetup{ghsystem/<option1>,ghsystem/<option2>}
```

## 34. Get Hazard and Precautionary Statements

### 34.1. Simple Statements

The general usage is simple: you use the command

► **\ghs\***[<options>]{<type>}{<number>}

There are three types available: h, euh and p. The {<type>} argument is case insensitive, so just type them in as you like.

```
1 \ghs{h}{200} \\
2 \ghs{H}{224} \\
3 \ghs{euh}{001} \\
4 \ghs{Euh}{202} \\
5 \ghs{p}{201}
```

The starred version hides the identifier and only gives the statement. If you want to hide the statement itself instead you can use the option:

► **hide** = true|false

There is an option to customize the output, too.

► **space** = <space command> → Space between <type> and <number>.

```
1 \ghs{h}{200} \\
2 \ghs[space=\,]{h}{200} \\
3 \ghs*{h}{200} \\
4 \ghs[hide]{h}{200}
```

### 34.2. Statements with Placeholders

Some of the statements contain placeholders. They can be one of the following:

- *<state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>*
- *<state specific effect if known>*
- *<or state all organs affected, if known>*
- *<name of sensitising substance>*

Except the last one which needs to be filled in, they are hidden per default. They can be made visible with the option

► `fill-in = true|false` → Show placeholders. Default = false

```

1  \ghs{h}{340} \\  

2  \ghs[fill-in]{h}{340} \\  

3  \ghs{h}{360} \\  

4  \ghs[fill-in]{h}{360} \\  

5  \ghs{h}{370} \\  

6  \ghs[fill-in]{h}{370} \\  

7  \ghs{euh}{208} \\  

8  \ghs[fill-in]{euh}{208}

```

These placeholders can be replaced with one of these options:

- `exposure = <text>` → exposure placeholder
- `effect = <text>` → effect placeholder
- `organs = <text>` → organ placeholder
- `substance = <text>` → substance placeholder

```

1  \ghs[exposure=This is how you get exposed.]{h}{340} \\  

2  \ghs[effect=These are the effects.]{h}{360} \\  

3  \ghs[organs=to this organ]{h}{370} \\  

4  \ghs[substance=substance]{euh}{208}

```



### 34.3. Statements with Gaps

Some of the statements have gaps that can be filled.

```
1 \ghs{p}{301} \\
2 \ghs{p}{401} \\
3 \ghs{p}{411} \\
4 \ghs{p}{413}
```

These gaps can be filled using these options:

- ▶ `text` = <text>
- ▶ `dots` = <text>
- ▶ `C-temperature` = <num>
- ▶ `F-temperature` = <num>
- ▶ `kg-mass` = <num>
- ▶ `lbs-mass` = <num>

```
1 \ghs[text=contact physician!]{p}{301} \\
2 \ghs[dots=here]{p}{401} \\
3 \ghs[C-temperature=50, F-temperature=122]{p}{411} \\
4 \ghs[kg-mass=5.0, lbs-mass=11, C-temperature=50, F-temperature=122]{p}{413}
```

### 34.4. Combined Statements

There are some combinations of statements. They are input with a + between the numbers:

```
1 \ghs{p}{235+410} \\
2 \ghs{p}{301+330+331}
```

Note that you can only get combinations that officially exist. *You can't combine freely.*

## 35. Pictograms

### 35.1. The Pictures

The GHS defines a number of pictograms:



The command

► `\ghspic[<options>]{<name>}`

loads them. Table 4 shows all available pictograms and their names. To be more precise: it shows the names to use with the `\ghspic` command. The file names are `ghsystem_<name>.<filetype>` where `<filetype>` is `eps`, `pdf`, `jpg` or `png`, see also section 35.2.

```
1 \ghspic{skull}
```



If you don't like the default size you can change it using this option:

► `scale = <factor>` → Scales the pictogram. Default = 1

The pictures are actually quite large. The default setting scales them by a factor of  $\frac{1}{20}$ .

```
1 \ghspic[scale=2]{skull}
```





If you want to use some specific `\includegraphics` options, e.g. if you want to rotate the pictogram for some reason, use this option:

► `includegraphics = {<includegraphics keyvals>}`


























```
1 \ghspic[includegraphics={angle=90}]{skull}
```







Table 4: All available GHS pictograms.

name	pictogram	name	pictogram
explos		explos-1	

35. Pictograms

name	pictogram	name	pictogram
explos-2		explos-3	
explos-4		explos-5	
explos-6			
flame		flame-2-white	
flame-2-black		flame-3-white	
flame-3-black		flame-4-1	
flame-4-2		flame-4-3-white	
flame-4-3-black		flame-5-2-white	
flame-5-2-black			
flame-0		flame-0-5-1	
bottle		bottle-2-black	
bottle-2-white			
acid		acid-8	
skull		skull-2	

name	pictogram	name	pictogram
skull-6			
exclam			
health			
aqpol			

### 35.2. Picture Type Depending on Engine

As you probably know you can't use every picture type with every compiler engine. pdf<sub>TEX</sub> in DVI mode *needs* eps pictures while pdf<sub>TEX</sub> in PDF mode, X<sub>Y</sub><sub>TEX</sub> and Lua<sub>TEX</sub> convert eps pictures into pdf files, given they have the rights to write in the directory the pictures are saved in.

However, the latter can include jpg and png without any problems, while pdf<sub>TEX</sub> in DVI mode can't.

To resolve this `GHSYSTEM` tests which engine is used and if pdf<sub>TEX</sub> which mode is used and then chooses either eps or pdf for the pictograms. You are free to choose the picture type yourself with the option

► `pic-type = eps|pdf|jpg|png`

## 36. Available Languages

Right now the H and P statements are only available in English, German or Italian. The package adapts the package option `german` but does not (yet) recognize language settings by `babel`<sup>35</sup> or `polyglossia`.<sup>36</sup>

You can also choose the language explicitly.

► `language = english|german|italian`

```

1  \ghs{h}{201}
2
3  \chemsetup[ghsystem]{language=german}
4  \ghs{h}{201}

```

I will add other languages some time in future. This may take a while, though. If you would be willing to contribute and write the statements of another language please feel free to contact me.<sup>37</sup> I would provide you with a template file, a pdf containing the official translations, and help to all your questions.

<sup>35</sup> CTAN: `babel`   <sup>36</sup> CTAN: `polyglossia`   <sup>37</sup> [contact@mychemistry.eu](mailto:contact@mychemistry.eu)

## 37. List of All Statements

If for some reason you want to list all sentences you can use

► `\ghslistall[<options>]`

This command has a number of options to customize the table, which is created with the `longtable` environment of the `longtable` package.

- `table-head-number` = <text> → Default = Identifier
- `table-head-text` = <text> → Default = Statement
- `table-next-page` = <text> → Default = continues on next page
- `table-caption` = <text> → As <text> in `\caption{<text>}`. Default = All H, EUH, and P Statements.
- `table-caption-short` = <text> → As <short> in `\caption[<short>]{<text>}`.
- `table-label` = <text> → The label to refer to the table with `\ref` and similar commands. Default = `tab:ghs-hp-statements`
- `table-row-sep` = <dim> → The separation of the table rows. A TeX dimension. Default = 3pt
- `table-rules` = `default`|`booktabs`|`none` → The style of the horizontal rules in the table. `default` uses `\hline`, `booktabs` uses `\toprule`, `\midrule` or `\bottomrule`, resp. This option needs the `booktabs`<sup>38</sup> package which you have to load yourself then. Default = `default`
- `table-top-head-rule` = `default`|`booktabs`|`none` → Change top rule explicitly. Default = `default`
- `table-head-rule` = `default`|`booktabs`|`none` → Change rule below head explicitly. Default = `default`
- `table-foot-rule` = `default`|`booktabs`|`none` → Change foot rule explicitly. Default = `default`
- `table-last-foot-rule` = `default`|`booktabs`|`none` → Change last foot rule explicitly. Default = `default`

The code below shows how table 5 was created:

```
1 \ghslistall[fill-in,table-rules=booktabs]
```

Table 5:

---



---



---

<sup>38</sup> CTAN: `booktabs`

---

---

# Part V.

## Appendix

### Overview: Options and Customization

#### Options

In the table below all options provided by CHEMMACROS for customization are listed. All options that belong to a module can be set with

► `\chemsetup[<module>]{<keyval>}` or

► `\chemsetup{<module>/<keyval>}`.

Some options can be set without value. Then the underlined value is used. The options belonging to the modules `chemformula` and `ghsystem` are not listed here.

option	module	values	default	
package options:				
<code>bpchem</code>	option	<u>true</u>  false	false	page 5
<code>circled</code>	option	formal  <u>all</u>  none	formal	page 5
<code>circletype</code>	option	chem math	chem	page 6
<code>cmversion</code>	option	1 2 bundle	bundle	page 6
<code>ghsystem</code>	option	<u>true</u>  false	true	page 6
<code>iupac</code>	option	auto restricted strict	auto	page 6
<code>language</code>	option	<language>	english	page 6
<code>method</code>	option	chemformula mhchem	chemformula	page 6
<code>Nu</code>	option	chemmacros mathspec	chemmacros	page 6
<code>strict</code>	option	<u>true</u>  false	false	page 6
<code>synchronize</code>	option	<u>true</u>  false	false	page 6
<code>greek</code>	option	math textgreek  <u>upgreek</u>	upgreek	page 6
<code>xspace</code>	option	<u>true</u>  false	true	page 6
<code>\ba, \Nu:</code>				
<code>elpair</code>	particle	<u>dots</u>  dash false	false	page 10
IUPAC commands:				
<code>break-space</code>	iupac	<dim>	.01em	page 12
<code>bridge-number</code>	iupac	sub super	sub	page 16
<code>cip-kern</code>	iupac	<dim>	.1ex	page 14
<code>coord-use-hyphen</code>	iupac	<u>true</u>  false	true	page 16
<code>hyphen-pre-space</code>	iupac	<dim>	.01em	page 12
<code>hyphen-post-space</code>	iupac	<dim>	-.03em	page 12
<code>\DeclareChemLatin:</code>				

Overview: Options and Customization

option	module	values	default	
<code>format</code>	<code>latin</code>	<code>&lt;anything&gt;</code>	<code>\itshape</code>	page 17
<code>\pch, \mch, \fpch, \fmch:</code>				
<code>append</code>	<code>charges</code>	<code>true false</code>	<code>false</code>	page 19
<code>acid/base:</code>				
<code>p-style</code>	<code>acid-base</code>	<code>slanted italics upright</code>	<code>upright</code>	page 18
<code>\ox:</code>				
<code>align</code>	<code>ox</code>	<code>center right</code>	<code>center</code>	page 20
<code>parse</code>	<code>ox</code>	<code>true false</code>	<code>true</code>	page 20
<code>roman</code>	<code>ox</code>	<code>true false</code>	<code>true</code>	page 20
<code>pos</code>	<code>ox</code>	<code>top super side</code>	<code>top</code>	page 20
<code>explicit-sign</code>	<code>ox</code>	<code>true false</code>	<code>false</code>	page 20
<code>decimal-marker</code>	<code>ox</code>	<code>comma point</code>	<code>point</code>	page 20
<code>\OX, \redox:</code>				
<code>dist</code>	<code>redox</code>	<code>&lt;dim&gt;</code>	<code>.6em</code>	page 23
<code>sep</code>	<code>redox</code>	<code>&lt;dim&gt;</code>	<code>.2em</code>	page 23
<code>\Enthalpy, \Entropy, \Gibbs:</code>				
<code>exponent</code>		<code>&lt;anything&gt;</code>	<code>\standardstate</code>	page 25
<code>delta</code>		<code>&lt;anything&gt; false</code>		page 25
<code>subscript</code>		<code>left right</code>		page 25
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## Commands

Quite a number of commands has been presented with which the possibilities of CHEMMACROS can be expanded. They are listed below for a quick overview.

- ▶ \DeclareChemArrow → Define new arrow, see page 56.
- ▶ \RenewChemArrow → Redefine existing arrow.
- ▶ \DeclareChemBond → Define a bond, see page 49.
- ▶ \RenewChemBond → Redefine a bond.
- ▶ \DeclareChemBondAlias → Declare an alias to an existing bond.
- ▶ \DeclareChemIUPAC → Define new IUPAC command, see page 16.
- ▶ \RenewChemIUPAC → Redefine IUPAC command.
- ▶ \DeclareChemLatin → Define new latin phrases, see page 17.
- ▶ \RenewChemLatin → Redefine latin phrases.
- ▶ \DeclareChemNMR → Define new NMR command, see page 28.
- ▶ \RenewChemNMR → Redefine NMR command.
- ▶ \DeclareChemParticle → Define new particle, see page 11.
- ▶ \RenewChemParticle → Redefine particle.
- ▶ \DeclareChemPhase → Define new phases command, see page 38.
- ▶ \RenewChemPhase → Redefine phases command.



- ▶ `\DeclareChemReaction` → Define new reaction environment, see page 35.
- ▶ `\DeclareChemState` → Define new state command, see page 26.
- ▶ `\RenewChemState` → Redefine state command.

## Suggestions and Bug Reports

Feedback on `CHEMMACROS`, `CHEMFORMULA` and `GHSYSTEM` is highly appreciated and welcome! Especially `CHEMFORMULA` and `GHSYSTEM` are still in beta testing phase so even if I repeat myself: feedback is highly welcome.

If you have suggestions for macros, missing features etc., please don't hesitate to contact me. If you recognize any errors, be it chemical ones, wrong documentation and the like, I'd be grateful about a short email.<sup>39</sup>

If you find any bugs, it would be best, if you'd send me a minimal example, with which I can reproduce the bug. You can also submit an issue on <https://bitbucket.org/cgnieder/chemmacros/> instead.

Many thanks to all the people who already provided me with feedback, especially (in alphabetical order):

- Peter Cao
- Christina Lüdigg
- Dr. Paul King
- Jonas Rivetti (Special thanks for his translation of the hazard and precautionary statements into Italian!)
- Christoph Schäfer
- Timo Stein

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<sup>39</sup> [contact@mychemistry.eu](mailto:contact@mychemistry.eu)

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Section titles are indicated  
**bold**, packages sans serif,  
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