the chemmacros bundle

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packages chemmacros, chemformula and ghsystem

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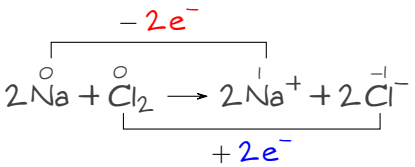
English documentation



Contents

Part I.
Preliminaries

1. Licence, Requirements and README

The CHEMMACROS bundle underlies the LaTeX 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[1] and l3packages.[2] It also needs the packages siunitx,[3] mathtools,[4] bm,[5] nicefrac[6] and environ[7] as well as tikz[8] and the Ti*k*Z libraries `calc` and `arrows`.

Package option `bpchem` (section 4) needs the package bpchem,[9] package option `xspace` needs the package xspace[10] and package option `method = mhchem` needs the package mhchem.[11]

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,[12] longtable,[13] ifpdf[14] and graphicx.[15] 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.

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

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 LaTeX 2ε 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[16] 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.

[16] This does not concern the `\ox` command. The IUPAC version is `\ox*`.

3. Installation, Loading the Bundle

The bundle comes with three style files,[17] 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

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

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

```
\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.

```
\usepackage{chemformula}
or
\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

```
\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

[17] Those ending sty.

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

option ▸ `circletype = chem|math` ⟶ This option switches between two kinds of circled charge symbols: `\fplus` ⨁ and `$\oplus$` ⊕. (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 = auto|math|textgreek|upgreek` ⟶ This Option determines how the letters `\Chemalpha` and friends are typeset. See page 10 for more information. *This option can only be chosen in the preamble.* Please note that this options *does not load either upgreek*[18] *nor textgreek*[19]! It only determines which one to choose if available. The option will detect if either upgreek or textgreek have been loaded and use them if available. If you explicitly choose `upgreek` or `textgreek` you also have to load the corresponding package. (default = `auto`)

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[20] 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 erros 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`)

[18] CTAN: upgreek [19] CTAN: textgreek [20] CTAN: mathspec

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.

- `\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`).

```
\chemsetup[option]{circled=none}\mch\ \pch\ \fmch\ \fpch\ \el\ \prt \\
\chemsetup[option]{circled=formal}\mch\ \pch\ \fmch\ \fpch\ \el\ \prt \\
\chemsetup[option]{circletype=math}\mch\ \pch\ \fmch\ \fpch\ \el\ \prt \\
\chemsetup{option/circletype=chem,option/circled=all}\mch\ \pch\ \fmch\ \fpch\ \
 el\ \prt \\
\chemsetup{option/circletype=math}\mch\ \pch\ \fmch\ \fpch\ \el\ \prt
```

$- + - + e^- p^+$
$- + \ominus \oplus e^- p^+$
$- + \circ \circ e^- p^+$
$\ominus \oplus \ominus \oplus e^{\ominus} p^{\oplus}$
$\circ \circ \circ \circ e^{\circ} p^{\circ}$

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

```
\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 50.
- New option `bond-style`, see page 50.
- 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.

- `\Hpl` ⟶ H^+ (proton)
- `\Hyd` ⟶ OH^- (hydroxide)
- `\HtO` ⟶ H_3O^+ (oxonium ion) (**H** three **O**)
- `\water` ⟶ H_2O
- `\el` ⟶ e^- (electron)
- `\prt` ⟶ p^+ (proton)
- `\ntr` ⟶ n^0 (neutron)
- `\Nu` ⟶ Nu^- (nucleophile). The package mathspec also defines a macro `\Nu`. If you chose package option `Nu = mathspec` CHEMMACROS defines `\Nuc` instead.
- `\El` ⟶ E^+ (electrophile)
- `\ba` ⟶ ba^- (base)
- `\fplus` ⟶ ⊕
- `\fminus` ⟶ ⊖
- `\transitionstatesymbol` ⟶ ‡

- \standardstate ⟶ ⦵. This symbol is only provided by CHEMMACROS, if the package chemstyle[21] is not loaded; the idea is borrowed from there.[22]
- \Chemalpha ⟶ α
- \Chembeta ⟶ β
- \Chemgamma ⟶ γ
- \Chemdelta ⟶ δ
- \Chemepsilon ⟶ ε
- \Chemeta ⟶ η
- \Chemkappa ⟶ κ
- \Chemmu ⟶ μ
- \Chemnu ⟶ ν
- \Chemrho ⟶ ρ
- \Chempi ⟶ π
- \Chemsigma ⟶ σ
- \Chemomega ⟶ ω
- \ChemDelta ⟶ Δ

> 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[23] is loaded, since it uses it's command \Lewis.

```
% needs package 'chemfig'
\ba[elpair] \Nu[elpair=dash]

\chemsetup[particle]{elpair}
\ba \Nu
```

ba:⁻ Nu|⁻
ba:⁻ Nu:⁻

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 package the letters are taken from there, and if you have loaded the package upgreek 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.

	math	upgreek	textgreek
\Chemalpha	α	α	α
\Chembeta	β	β	β
\ChemDelta	Δ	Δ	Δ

Table 1: The greek letters

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 partictle *will* obey the `circled` option.

```
% uses the 'upgreek' package
\DeclareChemParticle{\positron}{$\upbeta$+}
\DeclareChemParticle{\photon}{$\upgamma$}
\RenewChemParticle{\el}{$\upbeta$-}
\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.

[21] CTAN: chemstyle [22] many thanks to the package author Joseph Wright. [23] CTAN: chemfig

9. Nomenclature, Stereo Descriptors, Latin Phrases

9.1. IUPAC Names

Similar to the bpchem package CHEMMACROS provides a command[24] 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`.

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

Tetracyclo[2.2.2.1^{1,4}]-undecane-2-dodecyl-5-(heptadecylisododecylthioester)

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 a removes a small space after it. The command `\|` not only prevents ligatures but also inserts a small space.

```
\huge\iupac{2,4\-Di\|chlor\|pentan} \\
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` Ł) or are easily defined by another package or class (the cool[25] 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`.

[24] The idea and the implementation is shamelessly borrowed from bpchem by Bjørn Pedersen. [25] 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.

	auto	restricted	strict
`\L`	Ł	Ł	L
`\iupac{\L}`	L	L	L
`\D`	D	–	D
`\iupac{\D}`	D	D	D

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

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` ⟶ α
- `\b` ⟶ β
- `\g` ⟶ γ
- `\d` ⟶ δ
- `\k` ⟶ κ
- `\m` ⟶ μ
- `\n` ⟶ η
- `\w` ⟶ ω

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

5α-androstan-3β-ol
α-(trichloromethyl)-ω-chloropoly(1,4-phenylenemethylene)

Hetero Atoms and added Hydrogen Attachments to hetero atoms and added hydrogen atoms are indicated by italic letters [Coh+08]. CHEMMACROS defines a few shortcuts for the most common ones.

- `\H` ⟶ *H*
- `\O` ⟶ *O*
- `\N` ⟶ *N*
- `\Sf` ⟶ *S*
- `\P` ⟶ *P*

```
\iupac{\N\-methyl\|benz\|amide} \\
\iupac{3\H\-pyrrole} \\
\iupac{\O\-ethyl hexanethioate}
```

N-methylbenzamide
3*H*-pyrrole
O-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 (§) 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 = `.075em`

Fischer

- `\D` ⟶ D
- `\L` ⟶ L

Since the command `\L` has another meaning already (Ł) 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`: (R) `\Rconf[]`: ↻
- `\Sconf[<letter>]` ⟶ `\Sconf`: (S) `\Sconf[]`: ↻

Examples:

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

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

Coordination Chemistry

CHEMMACROS provides two commands useful with coordination chemistry:

- `\bridge{<num>}` ⟶ μ_3-
- `\hapto{<num>}` ⟶ η^5-

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

Ferrocene = bis(η^5-cyclopentadienyl)iron
tetra-μ_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.

```
\DeclareChemIUPAC\endo{\textit{endo}}
\RenewChemIUPAC\anti{\textit{anti}}
\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.

```
\iupac{\meta\-Xylol} \\
\RenewChemIUPAC\meta{\textit{m}}
\iupac{\meta\-Xylol}
```

m-Xylol
m-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*

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 abbremph.

The commands are defined through

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

```
\DeclareChemLatin\ltn{latin text}
\ltn
```

latin text

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^3 The units \cmc, \molar, and \Molar are defined by the package chemstyle as well. CHEMMACROS only defines them, if chemstyle is not loaded.
- \molar ⟶ $mol\,dm^{-3}$
- \moLar ⟶ $mol\,L^{-1}$
- \Molar ⟶ M
- \MolMass ⟶ $g\,mol^{-1}$
- \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

```
1  \Ka \Kb \pKa \pKa[1] \pKb \pKb[1]
```

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`

```
1  \pH, \pKa
2
3  \chemsetup[acid-base]{p-style=slanted} \pH, \pKa
4
5  \chemsetup[acid-base]{p-style=italics} \pH, \pKa
```

pH, pK_A
*p*H, pK_A
*p*H, pK_A

12. Oxidation Numbers, Real and Formal Charges

CHEMMACROS distinguishes between real (+/−) and formal (⊕/⊖) 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 (**p**lus + **ch**arge)
- `\mch[<number>]` ⟶ negative charge (**m**inus + **ch**arge)

```
\pch, Na\pch, Ca\pch[2]\\
\mch, F\mch, S\mch[2]
```

$^{+}$, Na^{+}, Ca^{2+}
$^{-}$, F^{-}, S^{2-}

The same for formal charges:

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

```
\fpch\ \fmch\ \fpch[3] \fmch[3]
```

$\oplus$ $\ominus$ $3\oplus$ $3\ominus$

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:

```
% uses package 'mhchem'
\chemsetup{charges/append=false,phases/pos=sub}
\ce{H\pch\aq} \ce{H\aq\pch}

\chemsetup[charges]{append=true}
\ce{H\pch\aq} \ce{H\aq\pch}
```

$H^{+}_{(aq)}$ $H^{+}_{(aq)}$
$H^{+}_{(aq)}$ $H_{(aq)}{}^{+}$

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):

```
\chemsetup{charges/append=false,phases/pos=sub}
\ce{\ox{1,H}\pch\aq}

\chemsetup[charges]{append=true}
\ce{\ox{1,H}\pch\aq}
```

$\overset{I}{H}{}^{+}_{(aq)}$
$\overset{I}{H}{}^{+}_{(aq)}$

12.2. Oxidation Numbers

Typesetting oxidation numbers:

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

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

$\overset{\mathrm{I}}{\mathrm{Na}}$, $\overset{\mathrm{II}}{\mathrm{Ca}}$, $\overset{-\mathrm{II}}{\mathrm{S}}$, $\overset{-\mathrm{I}}{\mathrm{F}}$

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 $\pm$ for 0. Default = `false`

ox ▸ `decimal-marker = comma|point` ⟶ choice for the decimal marker for formal oxidation numbers like $\overset{1.2}{\mathrm{X}}$. Default = `point`

ox ▸ `align = center|right` ⟶ center the oxidation number relative to the atom or right-align it. Default = `center`

```
\ox[roman=false]{2,Ca} \ox{2,Ca} \\
\ox[pos=super]{3,Fe}-Oxide \\
\ox[pos=side]{3,Fe}-Oxide \\
\ox[parse=false]{?,Mn} \\
\ox[align=right]{2,Ca}
```

$\overset{2}{\mathrm{Ca}}$ $\overset{\mathrm{II}}{\mathrm{Ca}}$
$\mathrm{Fe}^{\mathrm{III}}$-Oxide
Fe(III)-Oxide
$\overset{?}{\mathrm{Mn}}$
$\overset{\mathrm{II}}{\mathrm{Ca}}$

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

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

$\overset{\mathrm{III}}{\mathrm{Fe}}$ $\mathrm{Fe}^{\mathrm{III}}$

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

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

$\overset{+\mathrm{I}}{\mathrm{Na}}$, $\overset{+\mathrm{II}}{\mathrm{Ca}}$, $\overset{-\mathrm{II}}{\mathrm{S}}$, $\overset{\pm 0}{\mathrm{F}}_2$

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

Compare $\overset{-\mathrm{I}}{\mathrm{O}_2}^{2-}$ to $\overset{-\mathrm{I}}{\mathrm{O}_2}^{2-}$

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

```
\ox{.5,\ch{Br2}} \ch{"\ox{1/3,I}" {}3+}
```

The fraction uses the `\sfrac` command of the xfrac[26] package. For this purpose the instance `chemmacros-ox-frac` is defined.

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

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` ⟶ $\delta+$ (**del**ta + **p**lus)
- `\delm` ⟶ $\delta-$ (**del**ta + **m**inus)
- `\fdelp` ⟶ $\delta\oplus$
- `\fdelm` ⟶ $\delta\ominus$

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

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

The following macros are useful together with chemfig, too.

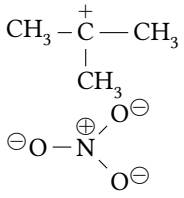
- `\scrp` ⟶ $+$ (**scr**iptstyle + **p**lus)
- `\scrm` ⟶ $-$ (**scr**iptstyle + **m**inus)
- `\fscrp` ⟶ $\oplus$

[26] CTAN: xfrac

- `\fscrm` ⟶ ⊖
- `\fsscrp` ⟶ ⊕ (using `\scriptscriptstyle`)
- `\fsscrm` ⟶ ⊖

```
\setatomsep{1.8em}\chemfig{CH_3-\chemabove{C}{\scrp}(-[6]C|H_3)-\vphantom{H_3}CH_3}

\chemfig{\fmch{}|O-\chemabove{N}{\fscrp}(-[1]O|\fmch)-[7]O|\fmch}
```



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 E1
- `\mech[e2]` ⟶ bimolecular elimination E2
- `\mech[cb]` ⟶ unimolecular elimination “conjugated base”, i.e. via carbanion $E1_{cb}$

14. Redox Reactions

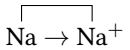
CHEMMACROS provides two commands to visualize the transfer of electrons in redox reactions. Both commands are using Ti*k*Z.

▸ `\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*.

```
\OX{a,Na} $\rightarrow$ \OX{b,Na}\pch\redox(a,b){oxidation}
```

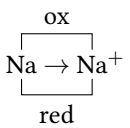


This line can be customized using Ti*k*Z keys in `[<tikz>]`:

```
\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.

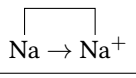
```
\OX{a,Na} $\rightarrow$ \OX{b,Na}\pch
\redox(a,b)[->,red]{ox}
\redox(a,b)[<-,blue][-1]{red}
\vspace{7mm}
```



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

redox ▸ `dist = <dim>` ⟶ A TEX dimension. Default = `.6em`

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

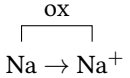


Additionally the option

redox ▸ `sep = <dim>` ⟶ Default = `.2em`

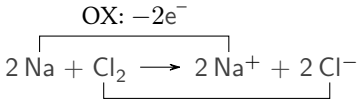
can be used to change the distance between the atom and the beginning of the line.

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

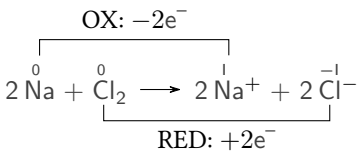


Examples:

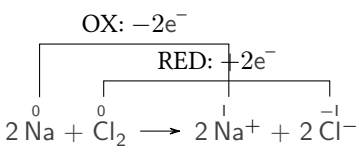
```
\ch{ 2 "\OX{o1,Na}" + "\OX{r1,Cl}" {}2 -> 2 "\OX{o2,Na}" \pch{} + 2
"\OX{r2,Cl}" \mch }
\redox(o1,o2){\small OX: $- 2\el$}
\redox(r1,r2)[][-1]{\small RED: $+ 2\el$}
\vspace{7mm}
```



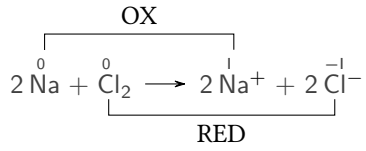

```
\ch{ 2 "\OX{o1,\ox{0,Na}}" + "\OX{r1,\ox{0,Cl}}" {}2 -> 2 "\OX{o2,\ox{+1,Na}}"
\pch{} + 2 "\OX{r2,\ox{-1,Cl}}" \mch }
\redox(o1,o2){\small OX: $- 2\el$}
\redox(r1,r2)[][-1]{\small RED: $+ 2\el$}
\vspace{7mm}
```




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



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



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:

```
\Enthalpy{123} \\
\Entropy{123} \\
\Gibbs{123}
```

$\Delta H^\ominus = 123\,\mathrm{kJ\,mol^{-1}}$
$S^\ominus = 123\,\mathrm{J\,K^{-1}\,mol^{-1}}$
$\Delta G^\ominus = 123\,\mathrm{kJ\,mol^{-1}}$

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

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.

```
\Enthalpy[unit=\kilo\joule]{-285} \\
\Gibbs[delta=false]{0} \\
\Entropy[delta=\Delta,exponent=]{56.7}
```

$\Delta H^\ominus = -285\,\mathrm{kJ}$
$G^\ominus = 0\,\mathrm{kJ\,mol^{-1}}$
$\Delta S = 56.7\,\mathrm{J\,K^{-1}\,mol^{-1}}$

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

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

$\Delta H^\ominus = -1234.56 \times 10^3\,\mathrm{kJ\,mol^{-1}}$
$\Delta H^\ominus = -1\,234{,}56 \cdot 10^3\,\mathrm{kJ/mol}$

15.1.1. Create New Variables

You can use the command

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

to create new corresponding commands:

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

$\Delta A^\ominus = 123.4\,\mathrm{kJ\,mol^{-1}}$
$\Delta E = -1.1\,\mathrm{V}$
$\Delta E^0_{\mathrm{Sn|Sn^{2+}||Pb^{2+}|Pb}} = 0.01\,\mathrm{V}$

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

▶ `exponent = <anything>`

▶ `delta = <anything>|false`

–none– ▶ `subscript-left = true|false`

▶ `subscript = <anything>`

15.1.2. Redefine Variables

With

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

you can redefine the already existing commands:

```
\RenewChemState{Enthalpy}{h}{\joule}
\Enthalpy(f){12.5}
```

$\Delta_\mathrm{f} h^\ominus = 12.5\,\mathrm{J}$

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:

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

$\Delta h = -12.3\,\mathrm{kJ\,mol^{-1}}\ \Delta H = -12.3\,\mathrm{kJ}$

15.2. State

The commands presented in section 15.1 internally all use the command[27]

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

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

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

$\Delta A^{\ominus}$, $\Delta_{\mathrm{f}} G^{\ominus}$, $\Delta E^{\ominus}_{\mathrm{Na}}$, $\Delta H^{1000\,^{\circ}\mathrm{C}}$

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:

^{1}H-NMR (400 MHz, $\mathrm{CDCl_3}$): δ = 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:

```
\NMR \\
\NMR*
```

^{1}H-NMR: δ
^{1}H-NMR

The first argument specifies the kind of NMR:

[27] Please note that `{<subscript>}` is an *optional* argument.

```
\NMR{13,C}
```
^{13}C-NMR: δ

The second argument sets the frequency (in MHz):

```
\NMR(400)
```
^{1}H-NMR (400 MHz): δ

You can choose another unit:

```
\NMR(4e8,\hertz)
```
^{1}H-NMR (4×10^{8} Hz): δ

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

```
\sisetup{exponent-product=\cdot}\NMR(4e8,\hertz)
```
^{1}H-NMR ($4 \cdot 10^{8}$ Hz): δ

The third argument specifies the solvent:

```
\NMR[CDCl3]
```
^{1}H-NMR ($CDCl_3$): δ

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>}`.

```
\DeclareChemNMR\HNMR{1,H}%
\DeclareChemNMR\CNMR{13,C}%
\CNMR*(100) \\
\HNMR*(400)
```
^{13}C-NMR (100 MHz)
^{1}H-NMR (400 MHz)

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]}` $^{13}C\{^1H\}$-NMR: δ
- `\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>}`

```
\begin{experimental}
 \data{type1} Data.
 \data{type2}[specifications] More data.
 \data*{type3} Even more data.
\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 be 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 δ.

`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 egual sign after `\NMR` and `\data`. Default = `false`

The default setup of the list:

```
    \topsep\z@skip \partopsep\z@skip
    \itemsep\z@ \parsep\z@ \itemindent\z@
    \leftmargin\z@
```

```
\begin{experimental}[format=\bfseries]
 \data{type1} Data.
 \data{type2}[specifications] More data.
 \data*{type3} Even more data.
\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.

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

type1 = Data. **type2 (specifications)** = More data. **^{1}H-NMR:** δ = 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.

```
\sisetup{separate-uncertainty,per-mode=symbol,detect-all,range-phrase=--}
\begin{experimental}[<optionen>]
 \data*{yield} \SI{17}{\milli\gram} yellow needles (\SI{0.04}{\milli\mole},
  \SI{13}{\percent}).
 %
 \data{mp.} \SI{277}{\celsius} (DSC).
 %
 \NMR(600)[CDCl3] \val{2.01} (s, \#{24}, \pos{5}), \val{2.31} (s, \#{12}, \
  pos{1}), \val{6.72--6.74} (m, \#{2}, \pos{11}), \val{6.82} (s, \#{8}, \pos
  {3}), \val{7.05--7.07} (m, \#{2}, \pos{12}), \val{7.39--7.41} (m, \#{4}, \
  pos{9}), \val{7.48--7.49} (m, \#{4}, \pos{8}).
 %
 \NMR{13,C}(150)[CDCl3] \val{21.2} ($+$, \#{4}, \pos{1}), \val{23.4} ($+$,
  \#{8}, \pos{5}), \val{126.0} ($+$, \#{4}, \pos{9}), \val{128.2} ($+$,
  \#{8}, \pos{3}), \val{130.8} ($+$, \#{2}, \pos{12}), \val{133.6} ($+$,
  \#{2}, \pos{11}), \val{137.0} ($+$, \#{4}, \pos{8}), \val{138.6} (q,
  \#{4}, \pos{2}), \val{140.6} (q, \#{2}, \pos{10}), \val{140.8} (q, \#{8},
  \pos{4}), \val{141.8} (q, \#{4}, \pos{6}), \val{145.6} (q, \#{2}, \pos{7})
  .
 %
 \data{MS}[DCP, EI, \SI{60}{\electronvolt}] \val{703} (2, \ch{M+}), \val
  {582} (1), \val{462} (1), \val{249} (13), \val{120} (41), \val{105} (100).
 %
```

```
\data{MS}[\ch{MeOH + H2O + KI}, ESI, \SI{10}{\electronvolt}] \val{720}
 (100, \ch{M+ + OH-}), \val{368} (\ch{M+ + 2 OH-}).
%
\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
 ).
%
\data*{UV-Vis} \SI{386}{\nano\metre} ($\varepsilon = \val{65984}$), \SI
 {406}{\nano\metre} ($\varepsilon = \val{65378}$).
%
\data*{quantum yield} $\Phi = \val{0.74+-0.1}$\,.
\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). ^{1}H-NMR (600 MHz, $CDCl_3$): 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). ^{13}C-NMR (150 MHz, $CDCl_3$): 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^+), 582 (1), 462 (1), 249 (13), 120 (41), 105 (100). MS (MeOH + H_2O + 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 (ε = 65 984), 406 nm (ε = 65 378). quantum yield: $\Phi = 0.74 \pm 0.10$.

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).
^{1}H-NMR (600 MHz, $CDCl_3$): 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).
^{13}C-NMR (150 MHz, $CDCl_3$): 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^+), 582 (1), 462 (1), 249 (13), 120 (41), 105 (100).
MS (MeOH + H_2O + 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 (ε = 65 984), 406 nm (ε = 65 378).
quantum yield: $\Phi = 0.74 \pm 0.10$.

16.5.3. Crazy

Output for these options: <optionen>:

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

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

mp. = 277 °C (DSC).

^{1}H-NMR (600 MHz, $CDCl_3$): δ $M^+ + H_2O$ = 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).

^{13}C-NMR (150 MHz, $CDCl_3$): δ $M^+ + H_2O$ = 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_2O + 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 (ε = 65 984), 406 nm (ε = 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.[28] It is meant to place text below of compounds.

[28] CHEMFORMULA provides its own possibility.

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

For example:

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

$$4\,C_2H_5Cl + Pb/Na \longrightarrow \underset{\substack{\text{former}\\ \text{antiknock}\\ \text{additive}}}{Pb(C_2H_5)_4} + NaCl$$

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`

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

$$4\,C_2H_5Cl + Pb/Na \longrightarrow \underset{\substack{\text{former}\\ \text{antiknock}\\ \text{additive}}}{Pb(C_2H_5)_4} + NaCl$$

$$4\,C_2H_5Cl + Pb/Na \longrightarrow \underset{\substack{\textbf{former}\\ \textbf{antiknock}\\ \textbf{additive}}}{Pb(C_2H_5)_4} + NaCl$$

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.

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

```
Reaction with counter:
\begin{reaction}
 A -> B
\end{reaction}
```

Reaction with counter:

$$A \longrightarrow B \tag{1}$$

```
Reaction without counter:
\begin{reaction*}
 C -> D
\end{reaction*}
```

Reaction without counter:

$$C \longrightarrow D$$

```
Several aligned reactions with counter:
\begin{reactions}
 A     &-> B + C \\
 D + E &-> F
\end{reactions}
```

Several aligned reactions with counter:

$$\begin{aligned} A &\longrightarrow B + C && (2)\\ D + E &\longrightarrow F && (3) \end{aligned}$$

```
Several aligned reactions without counter:
\begin{reactions*}
 G     &-> H + I \\
 J + K &-> L
\end{reactions*}
```

Several aligned reactions without counter:

$$\begin{aligned} G &\longrightarrow H + I\\ J + K &\longrightarrow L \end{aligned}$$

If you want to change the layout of the counter tags, you can use `\renewtagform{<tagname>}[<format>]{<right delim>}{<left delim>}`.[29]

```
\renewtagform{reaction}[R \textbf]{[}{]}
\begin{reaction}
 H2O + CO2 <<=> H2CO3
\end{reaction}
```

$$H_2O + CO_2 \rightleftharpoons H_2CO_3 \qquad [\mathrm{R}\ \mathbf{4}]$$

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

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

[29] Provided by the mathtools package

$$\mathrm{A} + 2\,\mathrm{B} \longrightarrow 3\,\mathrm{C} + \mathrm{D} \qquad \{5\}$$

Some text in between aligned reactions

$$3\,\mathrm{E} + \mathrm{F} \rightleftharpoons \mathrm{G} + \frac{1}{2}\,\mathrm{H} \qquad \{6\}$$

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 CHEMFORMULA/mhchem reactions. You could do the following:

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

With this the `reactionsat` environment is defined.

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

$$\mathrm{A} \longrightarrow \mathrm{B} \longrightarrow \mathrm{C} \longrightarrow \mathrm{D} \quad \{7\}$$
$$\mathrm{aaaaa} \longrightarrow \mathrm{bbbbb} \longrightarrow \mathrm{ccccc} \longrightarrow \mathrm{ddddd} \quad \{8\}$$

$$\mathrm{A} \longrightarrow \mathrm{B} \qquad \mathrm{C} \longrightarrow \mathrm{D}$$
$$\mathrm{aaaaa} \longrightarrow \mathrm{bbbbb} \qquad \mathrm{ccccc} \longrightarrow \mathrm{ddddd}$$

18.3. List of Reactions

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

▶ `\listofreactions`

```
\listofreactions
```

List of reactions

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.

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

$$2\,H_2O \rightleftharpoons H_3O^+ + OH^- \qquad \{9\}$$

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

- `\AddRxnDesc{<description>}`

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

$$Cl^{\bullet} + CH_4 \longrightarrow HCl + {}^{\bullet}CH_3 \qquad \{10\}$$
$$^{\bullet}CH_3 + Cl_2 \longrightarrow CH_3Cl + Cl^{\bullet} \qquad \{11\}$$

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 59.

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.

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

$C(s) + 2\,H_2O(l) \longrightarrow CO_2(g) + 2\,H_2(g)$
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.

> 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 TEX dimension. Default = `.1333em`

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

$\mathrm{C_{(s)} + 2\,H_2O_{(l)} \longrightarrow CO_{2(g)} + 2\,H_{2(g)}}$
To make it complete: $\mathrm{NaCl_{(aq)}}$.

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.

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

$\mathrm{NaOH\,(aq,\infty)\ H_2O\,(cd)\ U\,(cr)\ A\,(lc)}$
$\mathrm{NaOH_{(aq,\infty)}\ H_2O_{(cd)}\ U_{(cr)}\ A_{(lc)}}$

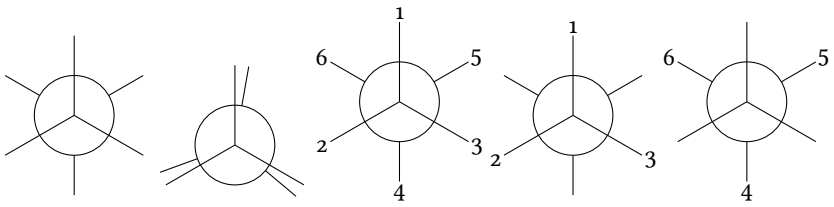
20. Newman Projections

CHEMMACROS provides the command

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

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

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



Several options allow customization:

`newman` ▸ `angle` = `<angle>` ⟶ default angle

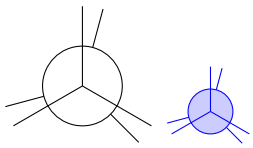
`newman` ▸ `scale` = `<factor>` ⟶ scale the whole projection

`newman` ▸ `ring` = `<tikz>` ⟶ customize the ring with Ti*k*Z keys

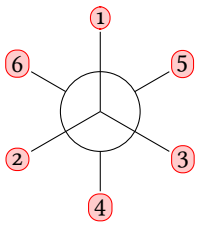
`newman` ▸ `atoms` = `<tikz>` ⟶ customize the nodes within which the atoms are set

`newman` ▸ `back-atoms` = `<tikz>` ⟶ explicitly customize the back atoms

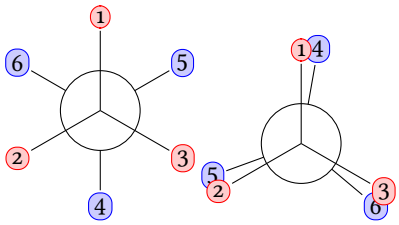
```
\chemsetup[newman]{angle=45} \newman{}
\newman[scale=.75,ring={draw=blue,fill=blue!20}]{}
```



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




```
\chemsetup[newman]{
  atoms = {draw=red,fill=red!20,inner sep=2pt,rounded corners},
  back-atoms = {draw=blue,fill=blue!20,inner sep=2pt,rounded corners}
}
\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`

`sp2`

`sp3`

```
\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)

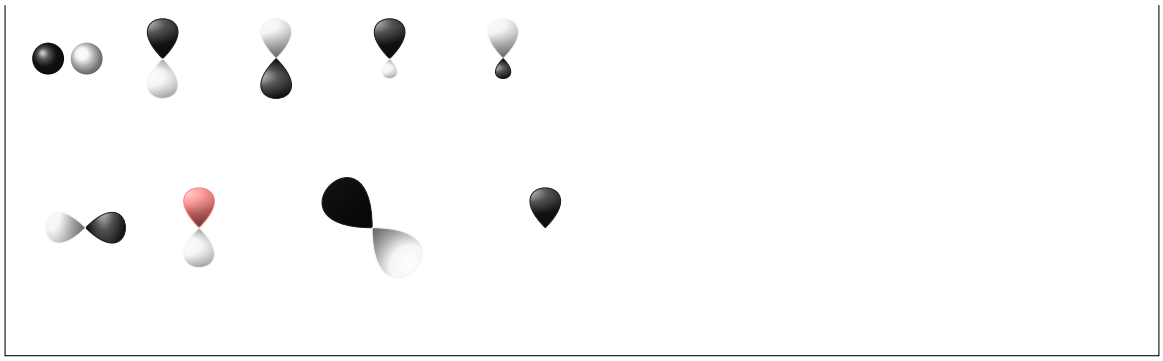
`orbital` ▸ `color` = `<color>` ⟶ changes the color of the orbital (all types)

`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`)

```
\orbital{s} \orbital[phase=-]{s}
\orbital{p} \orbital[phase=-]{p}
\orbital{sp3} \orbital[phase=-]{sp3}

\orbital[angle=0]{p} \orbital[color=red!50]{p} \orbital[angle=135,scale=1.5]{p}
 \orbital[half]{p}
```

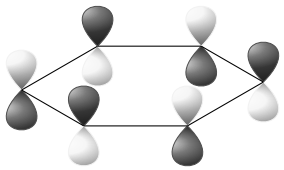


Additionally there are two options, with which the Ti*k*Z behaviour can be changed.

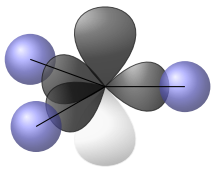
`orbital` ▸ `overlay` = `true`|`false` ⟶ the orbital "doesn't need space"; it is displayed with the Ti*k*Z option `overlay`.

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

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



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



Part III.
chemformula

22. Setup

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

```
\chemsetup[chemformula]{<options>} or
\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:

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

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

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

▶ `\ch{part1 part2 part3 part4}`

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

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

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

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

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

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

$\mathrm{{}_{2}H_2O}$
$\mathrm{2\,H_2O}$

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

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

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

24. Stoichiometric Factors

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

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

% decimals:
\ch{3.5} \\
\ch{5,75}

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

$\mathrm{2}$
$\mathrm{12}$
$\mathrm{3.5}$
$\mathrm{5.75}$
$\mathrm{\frac{3}{2}}$
$\mathrm{1\frac{1}{2}}$

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

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

If stoichiometric factors are enclosed with parentheses the fractions are not recognized. What's inside the parenthesis is typeset as is.

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

$\mathrm{(1/2)\,H_2O\ \tfrac{1}{2}\,H_2O\ 0.5\,H_2O}$

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

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

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 = <skip>` ⟶ The space that is placed after the stoichiometric factor. A rubber length. Default = `.1667em plus .0333em minus .0117em`

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

3,5 3·5

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

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

3⁄2 1½

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

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

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

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

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

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

3/2 1 1/2

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

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

$2\,H_2O$
$2\ H_2O$

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.

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

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

25.1. Adducts

CHEMFORMULA has two identifiers which will create adducts.

▶ `\ch{A.B}` ⟶

▶ `\ch{A*B}` ⟶

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

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

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

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

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

25.2. Subscripts

All numbers in a compound are treated as subscripts.

```
\ch{H2SO4}
```

H_2SO_4

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

```
\ch{A_nB_m}
```
$\ch{A_nB_m}$

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

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

25.3. Commands

Commands are allowed in a compound:

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

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

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

See section 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.

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

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

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

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

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

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

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

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

$\mathrm{H^{\oplus} + OH^{\ominus} \rightleftharpoons H_2O}$

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

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

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

- 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: $\mathrm{SO_4^{2-}}$, $\mathrm{(SO_4)^{2-}}$ 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":

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

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

Table 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

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.

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

C−C=C≡C⋯C⩬C≣C→C←C

Own Bonds CHEMFORMULA offers commands to define own bond types:

▸ \DeclareChemBond{<name>}{<code>}

▸ \RenewChemBond{<name>}{<code>}

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

▸ \ShowChemBond{<name>}

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

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

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

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

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

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

25.6. Customization

These options allow you to customize the ouptut 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 = `.25em`
- `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 = `.5833em`
- `bond-offset = <dim>` ⟶ Space between bond and atoms. Default = `.07em`
- `bond-style = <tikz>` ⟶ Ti*k*Z options for the bonds. Initially empty.
- `radical-style = <tikz>` ⟶ Ti*k*Z 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.

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

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

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

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

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

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

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

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

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

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

$M^{x+}\ SO_4^{2-}$
$M^{x+}\ SO_4^{2-}$

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

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

$H_2SO_4\ Na_3PO_4$
$H2SO4\ Na3PO4$
$H_2SO_4\ Na_3PO_4$

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

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

$A_nB_m\ H_2SO_4$
$A_nB_m\ H_2SO_4$

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

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

$Na_3PO_3 \cdot H_2O$
$Na_3PO_3 \cdot H_2O$

Changing the length of the bonds:

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

single: $CH_3—CH_3$
double: $CH_2═CH_2$
triple: CH≡CH

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

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

H−H + N≡N + O=O
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:

- `\ch{ + }` ⟶ `+` creates the plus sign between compounds with space around it: `\ch{2 Na + Cl2}` $2\,Na + Cl_2$
- `\ch{ v }` ⟶ ↓ sign for precipitate: `\ch{BaSO4 v}` $BaSO_4\downarrow$
- `\ch{ ^ }` ⟶ ↑ sign for escaping gas[30]: `\ch{H2 ^}` $H_2\uparrow$

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

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

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

A + B
A + B

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

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.

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

$H_2O + H_2SO_4 \longrightarrow H_3O^+ + HSO_4^-$
$H_2O + H2SO4 \longrightarrow H_3O^+ + HSO_4^-$

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

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

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

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

$H_2O + H2SO4 \longrightarrow H_3O^+ + HSO_4^-$
$H_2O + H2SO4 \longrightarrow H_3O^+ + HSO_4^-$

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>' }`

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

$\overset{II}{\mathrm{CaO}}$
$\ldots\mathrm{Na} + \ldots\mathrm{Cl_2} \longrightarrow \ldots\mathrm{NaCl}$
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{ $<escaped math>$ }`

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

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

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

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

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

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

28. Arrows

28.1. Arrow types

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

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

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

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

▸ `\ch{ </- }` ⟶ $\not\longleftarrow$ does not react (left)

▸ `\ch{ <-> }` ⟶ $\longleftrightarrow$ 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*k*Z.

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

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

28.2. Labels

The arrows take two optional arguments to label them.

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

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

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

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

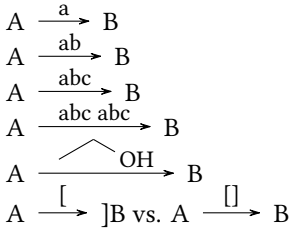
```
\ch{A ->[H2O] B} \\
\ch{A ->[ H2O ] B} \\
\ch{A ->[ "\ox{2,Ca}" F2 ] B} \\
\ch{A ->[$\Delta$,~ \[H+ \]] B}
```

$A \xrightarrow{H2O} B$
$A \xrightarrow[II]{H_2O} B$
$A \xrightarrow{CaF_2} B$
$A \xrightarrow{\Delta,\ [H^+]} B$

If you leave the blanks CHEMFORMULA treats the groups inside the square brackets as seperated input types. The arrow reads its arguments *afterwards*. As you can see the arrows "grow" with the

length of the labels. What stays constant is the part that protrudes the labels. As you also can see in the last example square brackets inside the arrow arguments should be produced using `\[` and `\]`. They keep their usual meaning outside `\ch`. These commands are necessary since the usual grouping (i.e. hiding the brackets inside curly brackets) doesn't work due to the way `\ch` reads its argument.

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



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 = `.75em`
- `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 $0.4\times$ the length of the longer arrow. Default = `.6`
- `compound-sep = <dim>` ⟶ The space between compounds and the arrows. Default = `.5em`
- `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 `<=>>` arrow:

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

standard: A $\underset{y}{\overset{x}{\rightleftharpoons}}$ B
longer: A $\underset{y}{\overset{x}{\longrightleftharpoons}}$ B
higher: A $\underset{y}{\overset{x}{\Longrightleftharpoons}}$ B
more balanced: A $\underset{y}{\overset{x}{\Longrightleftharpoons}}$ B
labels further away: A $\underset{y}{\overset{x}{\Longrightleftharpoons}}$ B
larger distance to compounds: A $\underset{y}{\overset{x}{\Longrightleftharpoons}}$ B
smaller labels: A $\underset{y}{\overset{x}{\Longrightleftharpoons}}$ 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

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

In order to define arrows yourself you need to know the basics of Ti*k*Z.[31] There are some predefined coordinates you can and should use:

`(cf_arrow_start)` The beginning of the arrow.

`(cf_arrow_end)` The end of the arrow.

`(cf_arrow_mid)` The mid of the arrow.

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

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

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

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

A ⋯▸ B A $\underset{b}{\overset{a}{\cdots\!\!\succ}}$ B A ⌒ B

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

▸ `\RenewChemArrow{<tokens>}{<tikz>}`

▸ `\ShowChemArrow{<tokens>}`

[31] Please see the pgfmanual for details.

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

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

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

A ⟶ 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:

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

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

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

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

$\underset{\text{water}}{H2O}$ $\underset{\text{water}}{H_2O}$ $\underset{2n-1}{H_2O}$ $\underset{H_2O}{H_2O}$ $\underset{\text{oxonium}}{H_3O^+}$

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

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

H2O (!)
A!()

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`

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

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

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:

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

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

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

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

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

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

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

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

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

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

▸ `format = <anything>` ⟶ Adds arbitrary code before the output of `\ch`.

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

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

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

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

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

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`.

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

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

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

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

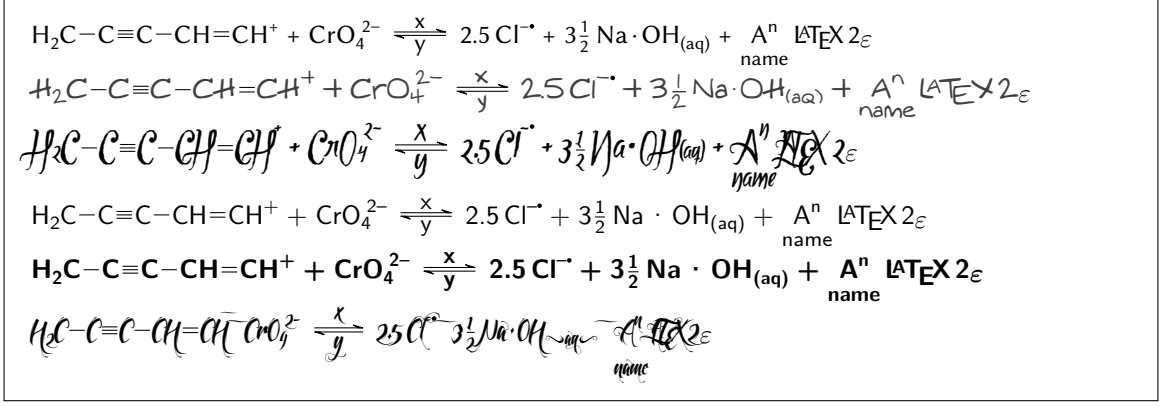
Hallo $H_2C-C\equiv C-CH=CH^+ + CrO_4^{2-} \rightleftharpoons[y]{x} 2.5\,Cl^{-\bullet} + 3\frac{1}{2}\,Na\cdot OH_{(aq)} + \underset{name}{A^n}\ LaTeX\,2\varepsilon$

If you're using XeLaTeX or LuaLaTeX and have loaded fontspec[32] you have the possibilty to set the font with it:

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

[32] CTAN: fontspec

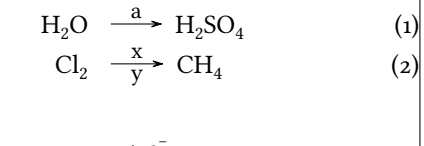
```
\chemsetup[chemformula]{font-spec={Linux Biolinum O}} \sample \\
\chemsetup[chemformula]{font-spec={[Color=darkgray]Augie}} \sample \\
\chemsetup[chemformula]{font-spec={Tipbrush Script}} \sample \\
\chemsetup[chemformula]{font-spec={Latin Modern Sans}} \sample \\
\bfseries \sample \normalfont \\
\chemsetup[chemformula]{font-spec={Feathergraphy Decoration}} \sample
```



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.

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



32. Further Examples

This section presents some examples of a possible usage.

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

$$\underset{\text{Synthesegas}}{n\,CO + (2n+1)\,H_2} \xrightarrow[[CoNi]]{200\,^{\circ}C} C_nH_{2n+2} + n\,H_2O \qquad \{12\}$$

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

a) $CH_4 + Cl_2 \longrightarrow CH_3Cl + HCl$ Chlormethan/Methylchlorid

b) $CH_3Cl + Cl_2 \longrightarrow CH_2Cl_2 + HCl$ Dichlormethan/Methylenchlorid

c) $CH_2Cl_2 + Cl_2 \longrightarrow CHCl_3 + HCl$ Trichlormethan/Chloroform

d) $CHCl_3 + Cl_2 \longrightarrow CCl_4 + HCl$ Tetrachlormethan/Tetrachlorkohlenstoff

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

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

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

	$CH_4(g)$	$+\ 2\,O_2(g)$	$\longrightarrow$	$CO_2(g) + H_2O(l)$	$+\ \Delta H^{\ominus}$
$\Delta_f H^{\ominus}$	??	0		$-94{\cdot}3 \quad -57{\cdot}9$	-192.1

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

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

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

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

$$\begin{aligned}
\ce{H3C-CH3 + Cl2 ->[\Delta][h\nu] H3CCH2Cl + HCl} \qquad & \Delta H = -27.1\,\mathrm{kJ} \\
\ce{H3C-CH3 + Cl^. -> H3CCH2^. + HCl} \qquad & \Delta H = -5.0\,\mathrm{kJ} \\
\ce{H3C-CH2^. + Cl2 -> H3CCH2Cl + Cl^.} \qquad & \Delta H = -23.0\,\mathrm{kJ}
\end{aligned}$$

The following example shows how the cancelling of compounds could be done.[33]

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

$$\begin{aligned}
\cancel{\ce{HCOOH(aq)}} + \ce{H2O(l)} &\rightleftharpoons \ce{H3O^+(aq)} + \cancel{\ce{HCOO^-(aq)}} \\
\cancel{\ce{HCOO^-(aq)}} + \ce{H2O(l)} &\rightleftharpoons \cancel{\ce{HCOOH(aq)}} + \ce{OH^-(aq)} \\
\hline
\ce{H2O(l)} + \ce{H2O(l)} &\rightleftharpoons \ce{H3O^+(aq)} + \ce{OH^-(aq)}
\end{aligned}$$

Part IV.
ghsystem

33. Setup

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

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

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

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.

```
\ghs{h}{200} \\
\ghs{H}{224} \\
\ghs{euh}{001} \\
\ghs{Euh}{202} \\
\ghs{p}{201}
```

H200: Unstable explosives.
H224: Extremely flammable liquid and vapour.
EUH001: Explosive when dry.
EUH202: Cyanoacrylate. Danger. Bonds skin and eyes in seconds. Keep out of the reach of children.
P201: Obtain special instructions before use.

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>`.

```
\ghs{h}{200} \\
\ghs[space=\,]{h}{200} \\
\ghs*{h}{200} \\
\ghs[hide]{h}{200}
```

H200: Unstable explosives.
H 200: Unstable explosives.
Unstable explosives.
H200

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`

```
\ghs{h}{340} \\
\ghs[fill-in]{h}{340} \\
\ghs{h}{360} \\
\ghs[fill-in]{h}{360} \\
\ghs{h}{370} \\
\ghs[fill-in]{h}{370} \\
\ghs{euh}{208} \\
\ghs[fill-in]{euh}{208}
```

H340: May cause genetic defects.
H340: May cause genetic defects. *<state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>*
H360: May damage fertility or the unborn child.
H360: May damage fertility or the unborn child. *<state specific effect if known> <state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>*
H370: Causes damage to organs.
H370: Causes damage to organs *<or state all organs affected, if known>*. *<state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>*
EUH208: Contains *<name of sensitising substance>*. May produce an allergic reaction.
EUH208: Contains *<name of sensitising substance>*. May produce an allergic reaction.

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

```
\ghs[exposure=This is how you get exposed.]{h}{340} \\
\ghs[effect=These are the effects.]{h}{360} \\
\ghs[organs=to this organ]{h}{370} \\
\ghs[substance=substance]{euh}{208}
```

H340: May cause genetic defects. This is how you get exposed.
H360: May damage fertility or the unborn child. These are the effects.
H370: Causes damage to this organ.
EUH208: Contains substance. May produce an allergic reaction.

34.3. Statements with Gaps

Some of the statements have gaps that can be filled.

```
\ghs{p}{301} \\
\ghs{p}{401} \\
\ghs{p}{411} \\
\ghs{p}{413}
```

P301: IF SWALLOWED:
P401: Store …
P411: Store at temperatures not exceeding ℃/°F.
P413: Store bulk masses greater than kg/lbs at temperatures not exceeding ℃/°F.

These gaps can be filled using these options:

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

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

P301: IF SWALLOWED: contact physician!
P401: Store here
P411: Store at temperatures not exceeding 50 °C/122 °F.
P413: Store bulk masses greater than 5.0 kg/11 lbs at temperatures not exceeding 50 °C/122 °F.

34.4. Combined Statements

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

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

P235 + P410: Keep cool. Protect from sunlight.
P301 + P330 + P331: IF SWALLOWED: rinse mouth. Do NOT induce vomitting.

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.

```
\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 $\frac{1}{20}$.

```
\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>}`

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

Table 4: All available GHS pictograms.

name	pictogram	name	pictogram
explos		explos-1	
explos-2		explos-3	
explos-4		explos-5	
explos-6			
flame		flame-2-white	
flame-2-black		flame-3-white	

name	pictogram	name	pictogram
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	
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. pdfTEX in DVI mode *needs* eps pictures while pdfTEX in PDF mode, XETEX and LuaTEX 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 pdfTEX in DVI mode can't.

To resolve this GHSYSTEM tests which engine is used and if pdfTEX 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[34] or polyglossia.[35]

You can also choose the language explicitly.

▶ language = english|german|italian

```
\ghs{h}{201}

\chemsetup[ghsystem]{language=german}
\ghs{h}{201}
```

H201: Explosive; mass explosion hazard.
H201: Explosiv, Gefahr der Massenexplosion.

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.[36] I would provide you with a template file, a PDF containing the official translations, and help to all your questions.

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>}.

[34] CTAN: babel [35] CTAN: polyglossia [36] contact@mychemistry.eu

- `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[37] 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:

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

Table 5: All H, EUH, and P Statements.

Identifier	Statement
H200	Unstable explosives.
H201	Explosive; mass explosion hazard.
H202	Explosive, severe projection hazard.
H203	Explosive; fire, blast or projection hazard.
H204	Fire or projection hazard.
H205	May mass explode in fire.
H220	Extremely flammable gas.
H221	Flammable gas.
H222	Extremely flammable aerosol.
H223	Flammable aerosol.
H224	Extremely flammable liquid and vapour.
H225	Highly flammable liquid and vapour.
H226	Flammable liquid and vapour.
H228	Flammable solid.
H240	Heating may cause an explosion.

continues on next page

[37] CTAN: booktabs

Identifier	Statement
H241	Heating may cause a fire or explosion.
H242	Heating may cause a fire.
H250	Catches fire spontaneously if exposed to air.
H251	Self-heating: may catch fire.
H252	Self-heating in large quantities; may catch fire.
H260	In contact with water releases flammable gases which may ignite spontaneously.
H261	In contact with water releases flammable gases.
H270	May cause or intensify fire; oxidiser.
H271	May cause fire or explosion; strong oxidiser.
H272	May intensify fire; oxidiser.
H280	Contains gas under pressure; may explode if heated.
H281	Contains refrigerated gas; may cause cryogenic burns or injury.
H290	May be corrosive to metals.
H300	Fatal if swallowed.
H301	Toxic if swallowed.
H302	Harmful if swallowed.
H304	May be fatal if swallowed and enters airways.
H310	Fatal in contact with skin.
H311	Toxic in contact with skin.
H312	Harmful in contact with skin.
H314	Causes severe skin burns and eye damage.
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H318	Causes serious eye damage.
H319	Causes serious eye irritation.
H330	Fatal if inhaled.
H331	Toxic if inhaled.
H332	Harmful if inhaled.
H334	May cause allergy or asthma symptoms orbreathing difficulties if inhaled.
H335	May cause respiratory irritation.
H336	May cause drowsiness or dizziness.
H340	May cause genetic defects. *<state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>*

continues on next page

Identifier	Statement
H341	Suspected of causing genetic defects. *<state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>*
H350	May cause cancer. *<state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>*
H351	Suspected of causing cancer. *<state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>*
H360	May damage fertility or the unborn child. *<state specific effect if known> <state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>*
H361	Suspected of damaging fertility or the unborn child. *<state specific effect if known> <state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>*
H362	May cause harm to breast-fed children.
H370	Causes damage to organs *<or state all organs affected, if known>. <state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>*
H371	May cause damage to organs *<or state all organs affected, if known>. <state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>*
H372	Causes damage to organs *<or state all organs affected, if known>* through prolonged or repeated exposure. *<state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>*
H373	May cause damage to organs *<or state all organs affected, if known>* through prolonged or repeated exposure. *<state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>*
H400	Very toxic to aquatic life.
H410	Very toxic to aquatic life with long lasting effects.
H411	Toxic to aquatic life with long lasting effects.
H412	Harmful to aquatic life with long lasting effects.
H413	May cause long lasting harmful effects to aquatic life.
H350i	May cause cancer by inhalation.
H360F	May damage fertility.
H360D	May damage the unborn child.
H361f	Suspected of damaging fertility.
H361d	Suspected of damaging the unborn child.

continues on next page

Identifier	Statement
H360FD	May damage fertility. May damage the unborn child.
H361fd	Suspected of damaging fertility. Suspected of damaging the unborn child.
H360Fd	May damage fertility. Suspected of damaging the unborn child.
H360Df	May damage the unborn child. Suspected of damaging fertility.
EUH001	Explosive when dry.
EUH006	Explosive with or without contact with air.
EUH014	Reacts violently with water.
EUH018	In use may form flammable/explosive vapour-air mixture.
EUH019	May form explosive peroxides.
EUH044	Risk of explosion if heated under confinement.
EUH029	Contact with water liberates toxic gas.
EUH031	Contact with acids liberates toxic gas.
EUH032	Contact with acids liberates very toxic gas.
EUH066	Repeated exposure may cause skin dryness or cracking.
EUH070	Toxic by eye contact.
EUH071	Corrosive to the respiratory tract.
EUH059	Hazardous to the ozone layer.
EUH201	Contains lead. Should not be used on surfaces liable to be chewed or sucked by children.
EUH201A	Warning! contains lead.
EUH202	Cyanoacrylate. Danger. Bonds skin and eyes in seconds. Keep out of the reach of children.
EUH203	Contains chromium(VI). May produce an allergic reaction.
EUH204	Contains isocyanates. May produce an allergic reaction.
EUH205	Contains epoxy constituents. May produce an allergic reaction.
EUH206	Warning! Do not use together with other products. May release dangerous gases (chlorine).
EUH207	Warning! Contains cadmium. Dangerous fumes are formed during use. See information supplied by the manufacturer. Comply with the safety instructions.
EUH208	Contains *<name of sensitising substance>*. May produce an allergic reaction.
EUH209	Can become highly flammable in use.
EUH209A	Can become flammable in use.
EUH210	Safety data sheet available on request.
EUH401	To avoid risks to human health and the environment, comply with the instructions for use.

continues on next page

Identifier	Statement
P101	If medical advice is needed, have product container or label at hand.
P102	Keep out of reach of children.
P103	Read label before use.
P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P210	Keep away from heat/sparks/open flames/hot surfaces. — No smoking.
P211	Do not spray on an open flame or other ignition source.
P220	Keep/Store away from clothing/…/combustible materials.
P221	Take any precaution to avoid mixing with combustibles …
P222	Do not allow contact with air.
P223	Keep away from any possible contact with water, because of violent reaction and possible flash fire.
P230	Keep wetted with …
P231	Handle under inert gas.
P232	Protect from moisture.
P233	Keep container tightly closed.
P234	Keep only in original container.
P235	Keep cool.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ventilating/lighting/… equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P244	Keep reduction valves free from grease and oil.
P250	Do not subject to grinding/shock/…/friction.
P251	Pressurized container: Do not pierce or burn, even after use.
P260	Do not breathe dust/fume/gas/mist/vapours/spray.
P261	Avoid breathing dust/fume/gas/mist/vapours/spray.
P262	Do not get in eyes, on skin, or on clothing.
P263	Avoid contact during pregnancy/while nursing.
P264	Wash … thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.

continues on next page

Identifier	Statement
P272	Contaminated work clothing should not be allowed out of the workplace.
P273	Avoid release to the environment.
P280	Wear protective gloves/protective clothing/eye protection/face protection.
P281	Use personal protective equipment as required.
P282	Wear cold insulating gloves/face shield/eye protection.
P283	Wear fire/flame resistant/retardant clothing.
P284	Wear respiratory protection.
P285	In case of inadequate ventilation wear respiratory protection.
P231 + P231	Handle under inert gas. Protect from moisture.
P235 + P410	Keep cool. Protect from sunlight.
P301	IF SWALLOWED:
P302	IF ON SKIN:
P303	IF ON SKIN (or hair):
P304	IF INHALED:
P305	IF IN EYES:
P306	IF ON CLOTHING:
P307	IF exposed:
P308	IF exposed or concerned:
P309	IF exposed or if you feel unwell:
P310	Immediately call a POISON CENTER or doctor/physician.
P311	Call a POISON CENTER or doctor/physician.
P312	Call a POISON CENTER or doctor/physician if you feel unwell.
P313	Get medical advice/attention.
P314	Get medical advice/attention if you feel unwell.
P315	Get immediate medical advice/attention.
P320	Spe cific treatment is urgent (see … on this label).
P321	Spe cific treatment (see … on this label).
P322	Spe cific measures (see … on this label).
P330	Rinse mouth.
P331	Do NOT induce vomitting.
P332	If skin irritation occurs:
P333	If skin irritation or rash occurs:
P334	Immerse in cool water/wrap in wet bandages.
P335	Brush off loose particles from skin.

continues on next page

Identifier	Statement
P336	Thaw frosted parts with lukewarm water. Do not rub affected area.
P337	If eye irritation persists:
P338	Remove contact lenses, if present and easy to do. Continue rinsing.
P340	Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P341	If breathing is difficult, remove victim to fresh air and keep at rest in a position comfortable for breathing.
P342	If experiencing respiratory symptoms:
P350	Gently wash with plenty of soap and water.
P351	Rinse cautiously with water for several minutes.
P352	Wash with plenty of soap and water.
P353	Rinse skin with water/shower.
P360	Rinse immediately contaminated clothing and skin with plenty of water before removing clothes.
P361	Remove/Take off immediately all contaminated clothing.
P362	Take off contaminated clothing and wash before reuse.
P363	Wash contaminated clothing before reuse.
P370	In case of fire:
P371	In case of major fire and large quantities:
P372	Explosion risk in case of fire.
P373	DO NOT fight fire when fire reaches explosives.
P374	Fight fire with normal precautions from a reasonable distance.
P375	Fight fire remotely due to the risk of explosion.
P376	Stop leak if safe to do so.
P377	Leaking gas fire: Do not extinguish, unless leak can be stopped safely.
P378	Use … for extinction.
P380	Evacuate area.
P381	Eliminate all ignition sources if safe to do so.
P390	Absorb spillage to prevent material damage.
P391	Collect spillage.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
P301 + P312	IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell.
P301 + P330 + P331	IF SWALLOWED: rinse mouth. Do NOT induce vomitting.

continues on next page

Identifier	Statement
P302 + P334	IF ON SKIN: Immerse in cool water/wrap in wet bandages.
P302 + P350	IF ON SKIN: Gently wash with plenty of soap and water.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P303 + P361 + P353	IF ON SKIN (or hair): Remove/Take off immediately all contaminated clothing. Rinse skin with water/shower.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P304 + P341	IF INHALED: If breathing is difficult, remove victim to fresh air and keep at rest in a position comfortable for breathing.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P306 + P360	IF ON CLOTHING: Rinse immediately contaminated clothing and skin with plenty of water before removing clothes.
P307 + P311	IF exposed: Call a POISON CENTER or doctor/physician.
P308 + P313	IF exposed or concerned: Get medical advice/attention.
P309 + P311	IF exposed or if you feel unwell: Call a POISON CENTER or doctor/physician.
P332 + P313	If skin irritation occurs: Get medical advice/attention.
P333 + P313	If skin irritation or rash occurs: Get medical advice/attention.
P335 + P334	Brush off loose particles from skin. Immerse in cool water/wrap in wet bandages.
P337 + P313	If eye irritation persists: Get medical advice/attention.
P342 + P311	If experiencing respiratory symptoms: Call a POISON CENTER or doctor/physician.
P370 + P376	In case of fire: Stop leak if safe to do so.
P370 + P378	In case of fire: Use … for extinction.
P370 + P380	In case of fire: Evacuate area.
P370 + P380 + P375	In case of fire: Evacuate area. Fight fire remotely due to the risk of explosion.
P371 + P380 + P375	In case of major fire and large quantities: Evacuate area. Fight fire remotely due to the risk of explosion.
P401	Store …
P402	Store in a dry place.
P403	Store in a well-ventilated place.
P404	Store in a closed container.
P405	Store locked up.

continues on next page

Identifier	Statement
P406	Store in corrosive resistant/... container with a resistant inner liner.
P407	Maintain air gap between stacks/pallets.
P410	Protect from sunlight.
P411	Store at temperatures not exceeding ℃/°F.
P412	Store at temperatures not exceeding 50 ℃/122 °F.
P413	Store bulk masses greater than kg/lbs at temperatures not exceeding ℃/°F.
P420	Store away from other materials.
P422	Store contents under ...
P402 + P404	Store in a dry place. Store in a closed container.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.
P410 + P403	Protect from sunlight. Store in a well-ventilated place.
P410 + P412	Protect from sunlight. Do not expose to temperatures exceeding 50 ℃/122 °F.
P411 + P235	Store at temperatures not exceeding ℃/°F . Keep cool.
P501	Dispose of contents/container to ...

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:			

option	module	values	default	
bpchem	option	true|false	false	page 5
circled	option	formal|all|none	formal	page 5
circletype	option	chem|math	chem	page 6
cmversion	option	1|2|bundle	bundle	page 6
ghsystem	option	true|false	true	page 6
iupac	option	auto|restricted|strict	auto	page 6
language	option	<language>	english	page 6
method	option	chemformula|mhchem	chemformula	page 6
Nu	option	chemmacros|mathspec	chemmacros	page 6
strict	option	true|false	false	page 6
synchronize	option	true|false	false	page 6
greek	option	math|textgreek|upgreek	upgreek	page 6
xspace	option	true|false	true	page 6
\ba, \Nu:				
elpair	particle	dots|dash|false	false	page 10
IUPAC commands:				
break-space	iupac	<dim>	.01em	page 12
bridge-number	iupac	sub|super	sub	page 16
cip-kern	iupac	<dim>	.075em	page 14
coord-use-hyphen	iupac	true|false	true	page 16
hyphen-pre-space	iupac	<dim>	.01em	page 12
hyphen-post-space	iupac	<dim>	-.03em	page 12
\DeclareChemLatin:				
format	latin	<anything>	\itshape	page 17
\pch, \mch, \fpch, \fmch:				
append	charges	true|false	false	page 19
acid/base:				
p-style	acid-base	slanted|italics|upright	upright	page 18
\ox:				
align	ox	center|right	center	page 20
parse	ox	true|false	true	page 20
roman	ox	true|false	true	page 20
pos	ox	top|super|side	top	page 20
explicit-sign	ox	true|false	false	page 20
decimal-marker	ox	comma|point	point	page 20
\OX, \redox:				
dist	redox	<dim>	.6em	page 23
sep	redox	<dim>	.2em	page 23
\Enthalpy, \Entropy, \Gibbs:				
exponent		<anything>	\standardstate	page 25
delta		<anything>|false		page 25
subscript		left|right		page 25
unit		<unit>		page 25
\DeclareChemState, \RenewChemState:				
exponent		<anything>	\standardstate	page 25
delta		<anything>|false		page 25
subscript		<anything>		page 25
subscript-left		true|false		page 26
\State:				
exponent	state	<anything>	\standardstate	page 27

option	module	values	default	
delta	state	<anything>|false		page 27
subscript-left	state	true|false		page 27
\NMR:				
unit	nmr	<unit>	\mega\hertz	page 29
nucleus	nmr	{<num>,<atom symbol>}	{1,H}	page 29
format	nmr	<anything>		page 29
pos-number	nmr	side|sub	side	page 29
coupling-unit	nmr	<unit>	\hertz	page 29
parse	nmr	true|false	true	page 29
delta	nmr	<anything>		page 29
list	nmr	true|false	false	page 29
list-setup	nmr		see text	page 29
use-equal	nmr	true|false	true	page 29
\DeclareChemReaction:				
star		true|false	false	page 35
arg		true|false	false	page 35
list-name	reaction	<anything>	List of reactions	page 36
list-entry	reaction	<anything>	Reaction	page 36
\mhName:				
align	mhName	<alignment>	\centering	page 33
format	mhName	<commands>		page 33
fontsize	mhName	<fontsize>	\tiny	page 33
width	mhName	<dim>		page 33
phases:				
pos	phases	side|sub	side	page 38
space	phases	<dim>	.1333em	page 38
\newman:				
angle	newman	<angle>	0	page 39
scale	newman	<factor>	1	page 39
ring	newman	<tikz>		page 39
atoms	newman	<tikz>		page 39
back-atoms	newman	<tikz>		page 39
\orbital <type> = s|p|sp|sp2|sp3:				
phase	orbital/<type>	+|-	+	page 40
scale	orbital/<type>	<factor>	1	page 40
color	orbital/<type>	<color>	black	page 40
angle	orbital/<type>	<angle>	90	page 40
half	orbital/p	true|false	false	page 40
overlay	orbital	true|false	false	page 41
opacity	ornital	<num>	1	page 41

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 57.
- \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.[38]

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 Lüdigk
- Dr. Paul King

[38] contact@mychemistry.eu

- Jonas Rivetti (Special thanks for his translation of the hazard and precautionary statements into Italian!)
- Christoph Schäfer
- Timo Stein

References

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Index

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