

# CHEMMACROS

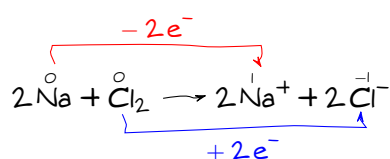
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comprehensive support for typesetting chemistry documents

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## Part I.

# Preliminaries

## 1. Licence, Requirements and README

Permission is granted to copy, distribute and/or modify this software under the terms of the L<sup>A</sup>T<sub>E</sub>X Project Public License (LPPL), version 1.3 or later (<http://www.latex-project.org/lppl.txt>). The software has the status “maintained.”

**CHEMMACROS** loads the packages expl3 [L3Pa] and xparse [L3Pb]. Depending on your usage other packages will be loaded. They are mentioned when the corresponding module using the package is described.

## 2. Motivation and Background

This package grew from a small collection of personal helper macros back in 2010 into a rather big package supporting various different chemical typesetting tasks. I hope I have achieved the following points with this package:

### 3. The Structure of **CHEMMACROS**

- Intuitive usage as far as the syntax of the commands is concerned.
- A comprehensive set of macros! If there are any needs you might have with respect to typesetting of chemistry which is not supported by this package<sup>1</sup> then let me know so **CHEMMACROS** can be extended.
- 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 `\textit{o}`-dichlorobenzene); the latter in my opinion also is more in the spirit of L<sup>A</sup>T<sub>E</sub>X 2<sub>ε</sub>.
- As much customizability as I could think of so every user can adapt the commands to his or her own wishes.
- Default settings that are 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 I would welcome an email<sup>2</sup> very much!

## 3. The Structure of **CHEMMACROS**

### 3.1. General Structure

Introduced in  
version 5.0

Since version 5.0 the **CHEMMACROS** package has a strictly modular structure. One the one hand this eases maintenance but it will also allow for easy and quick extension in the future. In a way it is a logical consequence from **CHEMMACROS**' history: since version 2.0, *i. e.*, since the fall of 2011 **CHEMMACROS** already had modular options.

The different modules of **CHEMMACROS** are divided into two groups:

1. Internal modules which provide underlying functionality or basic functionality which is not of direct interest from a user perspective.
2. User modules which provide all the stuff for typesetting.

Both groups each are subdivided into two groups: preloaded modules and modules which have to be loaded by the programmer (internal modules) or by the document author (user modules). Those modules are described in parts II and III of this manual.

The above means that not all functionality is available per default. If you want to load *all* modules no matter what then you can say:

```
1 \usechemmodule{all}
```

or

---

1. Not including needs already solved by other packages such as chemnum or chemfig.

2. See section B on page 58.

```
1 \chemsetup{modules=all}
```

which will load all modules which are part of **CHEMMACROS** (also see section 7.1). Own modules (see section A on page 57) are *not* loaded through this, though, and still have to be loaded additionally.

In part II the preloaded modules are described, first the user modules then the internal ones, in part III the other available modules are described, again the user modules first. In each section the modules are described in an alphabetical order.

### 3.2. Using **CHEMMACROS**' Options

Prior to v5.0 **CHEMMACROS** had quite a number of package options. **CHEMMACROS** v5.0 or higher has none! All of **CHEMMACROS**'s options are set using the command

```
\chemsetup[⟨module⟩]{⟨option list⟩}
CHEMMACROS' setup command.
```

When an option is described then in the left margin the module the option belongs to is denoted. This looks something like this:

```
module » option = {⟨value⟩} (initially empty)
```

Description of **option**. The module is printed in the left margin. The default value to the right is the setting the option has when **CHEMMACROS** is loaded. This can be an explicit setting but the option can also be empty.

```
module » choice-option = list|of|choices Default: list
```

Description of **choice-option**. A choice option can only be used with a predefined list of values. If one of the values is underlined it means that the option can be used without value in which case the underlined value is chosen. If no value is underlined then a value *has* to be given by the user.

```
module » boolean-option = true|false Default: true
```

Description of **boolean-option**. A boolean option is a choice option with exactly the two values true and false. If the option is called without value then the underlined value is chosen (which is always true for a boolean option).

An option or list of options belonging to a module `module` can be set in two ways:

```
1 % first possibility:
2 \chemsetup[module]{
3   option1 = value ,
4   option2 = value
5 }
6 % second possibility:
7 \chemsetup{
8   module/option1 = value ,
9   module/option2 = value
10 }
```

The second way allows to set options belonging to different modules with one call of `\chemsetup`.

### 3.3. Support Package **CHEMFORMULA**

**CHEMFORMULA** provides means of typesetting chemical formulæ and reactions. You'll will see its macros `\ch` and `\chcpd` every now and then in this manual. When using **CHEMMACROS** you can consider the **CHEMFORMULA** package [Nie15a] to be loaded as **CHEMMACROS** makes use of it in various places. **CHEMMACROS** and **CHEMFORMULA** are tightly intertwined. In fact: *when using **CHEMMACROS** you should prefer **CHEMFORMULA** over **mhchem** (which provides very similar functionality) for having consistent typesetting.*

A historical note: **CHEMFORMULA** started as a part of **CHEMMACROS** in January 2012. Since July 2013 it is a completely independent package – from **CHEMFORMULA**'s point of view. It is maintained independently and has a manual of its own.

### 3.4. Upgrading from version < 5.0

People upgrading from versions < 5.0 will find that almost everything they know from earlier versions is the same in versions  $\geq 5.0$ . But there are important and *breaking* differences:

- **CHEMMACROS** has no package options any more, all options are set via `\chemsetup`.
- Not all of the features are available per default any more, for some the corresponding module has to be loaded explicitly. If suddenly some commands or environments seem to be undefined this may be the reason.
- Some option modules have been renamed (e.g., `iupac` is now `nomenclature`). If you experience strange errors when you upgrade your document this is the most likely source.
- The command family `\NewChem...`, `\RenewChem...` and `\DeclareChem...` has a new member `\ProvideChem...`.
- The macro `\ox` has another default behaviour (`pos = {super}`) and the starred version has another effect (`pos = {top}`) than the same macro in earlier versions. Now the default behaviour follows IUPAC recommendations. A second change is that the atom is now treated as a **CHEMFORMULA** formula.
- The syntax of `\NewChemReaction` and friends is now different from what it used to be. If you have defined your own reaction environments you need to adapt!
- **CHEMMACROS** offers a macro `\state` which is similar to but different from the earlier macro `\State`. `\State` is deprecated. There are also differences in the syntax of `\enthalpy` vs. the earlier `\Enthalpy`, `\entropy` vs. `\Entropy` and `\gibbs` vs. `\Gibbs`. The uppercase versions are deprecated. The macro `\NewChemState` also has a different syntax now.
- At various places in the code improvements and fixes have been made, too many to list them here. You should keep an open eye and first of all read the manual closely.

### 3.5. Compatibility Mode

#### 3.5.1. For Users

It is actually not true that **CHEMMACROS**' has no package options any more. It has one very important package option:

`compatibility = {\num}`

Default: 5.0

Let's you specify the version of **CHEMMACROS** you want to use. Any number smaller than

### 3. The Structure of **CHEMMACROS**

5.0 will load v4.7. *i. e.*, the last version before **CHEMMACROS** got its modular structure. Not using the option will always load the newest version. Please note that you only can specify the *number* of the version. For a version “5.2c” you can only set compatibility mode “5.2” but not specify the subversion.

In your document you can check for the compatibility mode:

**\IfChemCompatibilityTF**{<comp>}{<num>}{<true>}{<false>}

Checks the value given through the option **compatibility** against <num> using <comp> and either leaves <true> or <false> in the input stream. <comp> can be one of <, <=, =, >= or >.

**\IfChemCompatibilityT**{<comp>}{<num>}{<true>}

Checks the value given through the option **compatibility** against <num> using <comp> and leaves <true> in the input stream if the check is logically true. <comp> can be one of <, <=, =, >= or >.

**\IfChemCompatibilityF**{<comp>}{<num>}{<false>}

Checks the value given through the option **compatibility** against <num> using <comp> and leaves <false> in the input stream if the check is logically false. <comp> can be one of <, <=, =, >= or >.

A possible check:

```
1 \IfChemCompatibilityT{>=}{5.0}{\usechemmodule{all}}
```

Loading **CHEMMACROS** with **compatibility** = {4.7} also allows to use the package options from that version:

```
1 \usepackage[compatibility=4.7,language=german]{chemmacros}
```

#### 3.5.2. For Module Writers

For future versions the aim is not to make such breaking changes again. While we never know what the future actually will bring **CHEMMACROS** now has the tools for tying code to a version number:

\* **\chemmacros\_if\_compatibility:nnTF** {<comp>} {<num>} {<true>} {<false>}  
expl3 version of **\IfChemCompatibilityTF**.

In modules one can try adding code for a certain version or range of versions:

**\ChemCompatibility**{<num>} <code> **\EndChemCompatibility**

Leaves <code> in the input stream if the compatibility version  $x$  given by **compatibility** matches <num> ( $x = \langle num \rangle$ ).

**\ChemCompatibilityFrom**{<num>} <code> **\EndChemCompatibility**

Leaves <code> in the input stream if the compatibility version  $x$  given by **compatibility** matches <num> or newer. This means <num> is the *oldest* version allowed ( $x \geq \langle num \rangle$ ).

## 4. General Options

`\ChemCompatibilityTo{<num>} <code> \EndChemCompatibility`

Leaves `<code>` in the input stream if the compatibility version  $x$  given by `compatibility` matches `<num>` or older. This means `<num>` is the *newest* version allowed ( $x \leq \langle num \rangle$ ).

`\ChemCompatibilityBetween{<num1>}{<num2>} <code> \EndChemCompatibility`

Leaves `<code>` in the input stream if the compatibility version  $x$  given by `compatibility` lies between `<num1>` and `<num2>` ( $\langle num1 \rangle \leq x \leq \langle num2 \rangle$ ).

`\EndChemCompatibility`

This macro *must* end each of the `\ChemCompatibility...` macros.

## 4. General Options

**CHEMMACROS** has some core options which don't belong to any of the modules described in parts II and III. Those options have no module denoted in the left margin next to their descriptions and are also set without specifying a module:

```
1 \chemsetup{
2   option1 = value ,
3   option2 = value
4 }
```

Two of those options are explained now:

`modules` = {<comma separated list of module names>} (initially empty)

With this option you can specify which modules you want to load. Alternatively you can use `\usechemmodule{<comma separated list of module names>}`.

`greek` = {<mapping>} (initially empty)

Explicitly specify which mapping should be used by the **CHEMGREEK** package [Nie15b]. For details about what this means please refer to section 6.3 on page 24.

Some internal modules may also define core options, *e.g.*, the `lang` module, see section 6.4 on page 25.

## Part II.

# The Preloaded Modules

## 5. User Modules

### 5.1. The acid-base Module

Easy representation of pH,  $pK_a$ ...

`\pH`  
pH

`\pOH`  
 $pOH$

`\Ka`  
 $K_a$ , depends on language settings, see section 6.4. The translations can be adapted.

`\Kb`  
 $K_b$

`\Kw`  
 $K_w$

`\pKa[⟨num⟩]`  
`\pKa`:  $pK_a$ , `\pKa[1]`:  $pK_{a1}$ , depends on language settings, see section 6.4. The translations can be adapted.

`\pKb[⟨num⟩]`  
`\pKb`:  $pK_b$ , `\pKb[1]`:  $pK_{b1}$

`\p{⟨anything⟩}`  
*e. g.* `\p{\Kw}`  $pK_w$

`\Ka` `\Kb` `\pKa` `\pKa[1]` `\pKb` `\pKb[1]`  $K_a$   $K_b$   $pK_a$   $pK_{a1}$   $pK_b$   $pK_{b1}$

The operator  $p$  [...] shall be printed in Roman type.

The IUPAC Green Book [Coh+08, p. 103]

There is one option which changes the style the  $p$  is typeset, other options allow to change the subscript of the constants:

`acid-base` » `p-style = italics|slanted|upright` Default: upright  
 Set the style of the  $p$  operator.

`acid-base` » `K-acid = {⟨text⟩}` Default: `\ChemTranslate{K-acid}`  
 The subscript to `\Ka` and `\pKa`.

`acid-base` » `K-base = {⟨text⟩}` Default: `\ChemTranslate{K-base}`  
 The subscript to `\Kb` and `\pKb`.

`acid-base` » `K-water = {⟨text⟩}` Default: `\ChemTranslate{K-water}`  
 The subscript to `\Kw`.

`\pH`, `\pKa` `\par`  
`\chemsetup[acid-base]{p-style=slanted} \pH`, `\pKa` `\par`  
`\chemsetup[acid-base]{p-style=italics} \pH`, `\pKa`

---

$pH$ ,  $pK_a$



$pH$ ,  $pK_a$   
 $pH$ ,  $pK_a$

As you can see the default subscripts of `\Kw`, `\Ka` and `\Kb` are lowercase letters. The literature is inconclusive about if this is the right way or if uppercase letters should be preferred. In textbooks the uppercase variant usually seems to be used while journals seem to prefer the lowercase variant. **CHEMMACROS**' default follows the usage in *The IUPAC Green Book* [Coh+08]. If you want to change this you have two possibilities:

```

1 % this works only in the preamble:
2 % \DeclareTranslation{English}{K-acid}{\mathrm{A}}% use your language here
3 % alternative:
4 \chemsetup{acid-base/K-acid=\mathrm{A}}% overwrites language dependent settings
5 \pKa

```

---

$pK_A$

## 5.2. The charges Module

The charges module loads the module `chemformula`.

### 5.2.1. Charge Symbols

`\fplus`

⊕ formal positive charge

`\fminus`

⊖ formal negative charge

`\scrip`

+ scriptstyle positive charge for usage in chemfig's [Tel13] formulas.

`\scrm`

- scriptstyle negative charge for usage in chemfig's formulas.

`\fscrp`

⊕ scriptstyle formal positive charge for usage in chemfig's formulas.

`\fscrm`

⊖ scriptstyle formal negative charge for usage in chemfig's formulas.

`\fsscrp`

⊕ scriptscriptstyle formal positive charge for usage in chemfig's formulas.

`\fsscrm`

⊖ scriptscriptstyle formal negative charge for usage in chemfig's formulas.

## 5.2.2. Ion Charges

Simple displaying of (real) charges. It is worth noting that these commands really are relicts from a time when `CHEMMACROS` tried hard to be compliant with `mhchem` and `CHEMFORMULA` didn't exist, yet. They are still provided for backwards compatibility but *my recommendation is to use `\ch`* (see the documentation of the `CHEMFORMULA` package [Nie15a]) *and forget about these commands:*

`\pch[⟨number⟩]`  
positive charge

`\mch[⟨number⟩]`  
negative charge

`\fpch[⟨number⟩]`  
formal positive charge

`\fmch[⟨number⟩]`  
formal negative charge

```
1 A\pch\ B\mch[3] C\fpch[2] D\fmch      A+ B3- C2⊕ D⊖
```

## 5.2.3. Partial Charges and Similar Stuff

The next ones probably are seldomly needed but nevertheless useful:

`\delp`  
 $\delta^+$  partial positive charge

`\delm`  
 $\delta^-$  partial negative charge

`\fdelp`  
 $\delta^\oplus$  partial formal positive charge

`\fdelm`  
 $\delta^\ominus$  partial formal negative charge

These macros for example can be used with the `\ox` command (see section 7.7) or with the `chemfig` package:

```
1 \chemsetup{
2   charges/circled = all,
3   redox/parse     = false,
4   redox/pos       = top
5 }
6 \ch{"\ox{\delp,H}" -{} "\ox{\delm,Cl}"} \hspace*{1cm}
7 \chemfig{\chemabove[3pt]{\lewis{246,Br}}{\delm}-\chemabove[3pt]{H}{\delp}}
```



### 5.2.4. Charge Options

`charges` » `circled` = `formal|all|none` Default: `formal`

**CHEMMACROS** uses two different kinds of charges which indicate the usage of real (+/−) and formal (⊕/⊖) charges. The option `formal` distinguishes between them, option `none` displays them all without circle, option `all` circles all.

`charges` » `circletype` = `chem|math` Default: `chem`

This option switches between two kinds of circled charge symbols: `\fpplus` ⊕/`\fminus` ⊖ (`chem`) and `\oplus` ⊕/`\ominus` ⊖ (`math`).

`charges` » `partial-format` = `{⟨LATEX code⟩}` Default: `\tiny`

Code which formats the macros defined with `\NewChemPartialCharge` (see section 5.2.5).

### 5.2.5. Own Charge Macros

Just in case the existing macros don't fit your needs there are commands for defining new ones or modifying the existing ones. These commands define macros like those described in section 5.2.2.

`\NewChemCharge{⟨cs⟩}{⟨charge symbol⟩}`

Defines a new macro `⟨cs⟩`. Raises an error if `⟨cs⟩` already exists.

`\RenewChemCharge{⟨cs⟩}{⟨charge symbol⟩}`

Redefines a new macro `⟨cs⟩`. Raises an error if `⟨cs⟩` doesn't exist.

`\DeclareChemCharge{⟨cs⟩}{⟨charge symbol⟩}`

Defines a macro `⟨cs⟩`. Silently overwrites `⟨cs⟩` if it exists.

`\ProvideChemCharge{⟨cs⟩}{⟨charge symbol⟩}`

Defines a new macro `⟨cs⟩`. Does nothing if `⟨cs⟩` already exists.

An example of usage is the definition of the existing ion charge macros:

```
1 \NewChemCharge\fpch{\fpplus}
2 \NewChemCharge\fmch{\fminus}
```

These commands define macros like those described in section 5.2.3.

`\NewChemPartialCharge{⟨cs⟩}{⟨charge symbol⟩}`

Defines a new macro `⟨cs⟩`. Raises an error if `⟨cs⟩` already exists.

`\RenewChemPartialCharge{⟨cs⟩}{⟨charge symbol⟩}`

Redefines a new macro `⟨cs⟩`. Raises an error if `⟨cs⟩` doesn't exist.

`\DeclareChemPartialCharge{⟨cs⟩}{⟨charge symbol⟩}`

Defines a macro `⟨cs⟩`. Silently overwrites `⟨cs⟩` if it exists.

`\ProvideChemPartialCharge{<cs>}{<charge symbol>}`

Defines a new macro <cs>. Does nothing if <cs> already exists.

An example of usage is the definition of the existing partial charge macros:

```
1 \NewChemPartialCharge\fdelp{\fplus}
2 \NewChemPartialCharge\fdelm{\fminus}
```

### 5.3. The nomenclature Module

The nomenclature module loads the tikz module. It also loads the package scrfile which is part of the KOMA-Script bundle [Koh15].

#### 5.3.1. The `\iupac` Command

Similar to the bpchem package [Pedo4] `CHEMMACROS` provides a command<sup>3</sup> to typeset IUPAC names. Why is that useful? IUPAC names can get very long. So long indeed that they span over more than two lines, especially in two-column documents. This means they must be allowed to be broken more than one time. This is what the following command does.

`\iupac{<IUPAC name>}`

Inside this command use | and \- to indicate a breaking point or a breaking dash. Use ^ as a shortcut for `\textsuperscript`.

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

---

Tetracyclo[2.2.2.1<sup>1,4</sup>]-undecane-2-dodecyl-5-(heptadecylisododecyl-thioester)

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 ^ without `\iupac`.

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

---

3. The idea and initial implementation is shamelessly borrowed from bpchem by Bjørn PEDERSEN.

TABLE 1: Demonstration of `iupac`'s modes.

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

```

1 \huge\iupac{2,4\Di|chlor|pentan} \par
2 2,4-Dichloropentan

```

2,4-Dichloropentan

2,4-Dichloropentan

The spaces inserted by `\-` and `|` can be customized.

`nomenclature` » `hyphen-pre-space = {<dim>}` Default: .01em

Set the space that is inserted before the hyphen set with `\-`.

`nomenclature` » `hyphen-post-space = {<dim>}` Default: - .03em

Set the space that is inserted after the hyphen set with `\-`.

`nomenclature` » `break-space = {<dim>}` Default: .01em

Set the space inserted by `|`.

The command `\iupac` serves another purpose, too, however. Regardless of the setting of the `iupac` option (see below) 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.<sup>4</sup> This means they either are predefined already (`\L` `L`) or are easily defined by another package or class (the cool package defines both `\D` and `\E`, for example). In order to give you control which commands are defined in which way, there is the option `iupac`:

`nomenclature` » `iupac = auto|restricted|strict` Default: auto

Take care of how IUPAC naming commands are defined.

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`.
- `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 1 demonstrates the different modes.

4. Please read section 5.3.2 before you consider using the one-letter commands

TABLE 2: IUPAC shortcuts for Greek letters.

macro	<code>\a</code>	<code>\b</code>	<code>\g</code>	<code>\d</code>	<code>\k</code>	<code>\m</code>	<code>\n</code>	<code>\w</code>
letter	$\alpha$	$\beta$	$\gamma$	$\delta$	$\kappa$	$\mu$	$\eta$	$\omega$

**5.3.2. Macros Defined (Not Only) For Usage in `\iupac`**

**One-letter Macros** For some of the macros explained in this section one-letter commands are defined – with a *caveat* in mind, though: they are not actively recommended. One-letter commands seldomly have meaningful names and often they’ve also been defined by other packages. This means they make collaboration more difficult than it needs to be and are a source for package conflicts. **CHEMMACROS** solves the latter problem by only providing them inside the argument of `\iupac`. The one exception **CHEMMACROS** makes is the command `\p` (for things like pH) which is and will remain an official command (see section 5.1). For all other one-letter macros alternatives with more meaningful names exist.

**Greek Letters** Greek letters in compound names are typeset upright. Here are a few examples for the existing macros:

`\chemalpha`  $\alpha$   
Upright lowercase alpha

`\chembeta`  $\beta$   
Upright lowercase alpha

`\chemgamma`  $\gamma$   
Upright lowercase alpha

`\chemdelta`  $\delta$   
Upright lowercase alpha

There exist two commands for each of the twenty-four Greek letters: a lowercase and an uppercase version (`\chemalpha` and `\chemAlpha`). Those commands are actually provided by the **CHEMGREEK** package. For more details read section 6.3 and also refer to **CHEMGREEK**’s documentation.

There are a number of one-letter commands that some people may find convenient to use which use above mentioned commands to print Greek letters inside `\iupac`. They’re listed in table 2.

```

1 \iupac{5\chemalpha\androstano-3\chembeta-ol} \par
2 \iupac{\chemalpha-(tri|chloro|methyl)-\chemomega
3 \-chloro|poly(1,4\phenylene|methylene)}
```

---

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

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

**\hydrogen** *H*

The italic H for hydrogen. (An alias for this command is **\H**.)

**\oxygen** *O*

The italic O for oxygen. (An alias for this command is **\O**.)

**\nitrogen** *N*

The italic N for nitrogen. (An alias for this command is **\N**.)

**\sulfur** *S*

The italic S for sulfur. (An alias for this command is **\Sf**.)

**\phosphorus** *P*

The italic P for phosphorus. (An alias for this command is **\P**.)

1 <b>\iupac</b> {\nitrogen\ -methyl  benz  amide}	<i>N</i> -methylbenzamide
2	
3 <b>\iupac</b> {3\hydrogen\ -pyrrole}	3 <i>H</i> -pyrrole
4	
5 <b>\iupac</b> {\oxygen\ -ethyl hexanethioate}	<i>O</i> -ethyl hexanethioate

### Cahn-Ingold-Prelog

**\cip**{<conf>}

Typeset Cahn-Ingol-Prelog descriptors, *e. g.*: **\cip**{R,S} (*R,S*)

**\rectus** (*R*)

Typeset rectus descriptor. (An alias for this command is **\R**.)

**\sinister** (*S*)

Typeset sinister descriptor. (An alias for this command is **\S**.)

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:

**nomenclature** » **cip-kern** = {<dim>}

Default: .075em

Set the amount of kerning after the closing parenthesis.

### Fischer

**\dexter** *D*

Typeset dexter descriptor. (An alias for this command is **\D**.)

**\laevus** *L*

Typeset laevus descriptor. (An alias for this command is **\L**.)

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

- `\cis cis` `\trans trans`
- `\fac fac` `\mer mer`
- `\sin sin` `\ter ter`
- `\zusammen (Z)` `\entgegen (E)`
- `\syn syn` `\anti anti`
- `\tert tert`

An alias for `\entgegen` is `\E` and an alias for `\zusammen` is `\Z`.



**ortho/meta/para**



`\ortho o` `\meta m` `\para p`

Although these commands are provided I like to cite *The IUPAC Blue Book* [PPRo4]:

The letters *o*, *m*, and *p* have been used in place of *ortho*, *meta*, and *para*, respectively, to designate the 1,2-, 1,3-, and 1,4- isomers of disubstituted benzene. This usage is strongly discouraged and is not used in preferred IUPAC names. [PPRo4, p. 90]

**Absolute Configuration**

`\Rconf[⟨letter⟩]`  
`\Rconf:`  `\Rconf[:]` 

`\Sconf[⟨letter⟩]`  
`\Sconf:`  `\Sconf[:]` 

**Coordination Chemistry** `CHEMMACROS` provides a few commands useful in coordination chemistry:

`\bridge{⟨num⟩}`  $\mu_3$ -  
 Denote bridging ligand connection.

`\hapto{⟨num⟩}`  $\eta^5$ -  
 Denote hapticity.

`\dento{⟨num⟩}`  $\kappa^2$ -  
 Denote denticity.

```
1 Ferrocene = \iupac{bis(\hapto{5}cyclopentadienyl)iron} \par
2 \iupac{tetra\-\bridge{3}iodido\-\tetrakis[tri|methyl|platinum(IV)]}
```

---

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



Two options allow customization:

- `nomenclature` » `bridge-number` = `sub`|`super` Default: `sub`  
 Appends the number as a subscript or superscript. IUPAC recommendation is the subscript [Con+05].
- `nomenclature` » `coord-use-hyphen` = `true`|`false` Default: `true`  
 Append a hyphen to `\hapto`, `\dent` and `\bridge` or don't.

### Examples

```

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

#### 5.3.3. Own `\iupac` Macros

If you find any commands missing you can define them using

`\NewChemIUPAC{<cs>}{<declaration>}`

Define a new IUPAC command that is in any case defined inside of `\iupac` regardless if `<cs>` is defined elsewhere already.

`\ProvideChemIUPAC{<cs>}{<declaration>}`

Define a new IUPAC command that is in any case defined inside of `\iupac` regardless if `<cs>` is defined elsewhere already only if the corresponding IUPAC macro is not defined, yet.

`\RenewChemIUPAC{<cs>}{<declaration>}`

Redefine an existing IUPAC command that is in any case defined inside of `\iupac` regardless if `<cs>` is defined elsewhere already.

`\DeclareChemIUPAC{<cs>}{<declaration>}`

Define a new IUPAC command that is in any case defined inside of `\iupac` regardless if `<cs>` is defined elsewhere already. This silently overwrites an existing IUPAC macro definition.

`\LetChemIUPAC{<cs1>}{<cs2>}`

Defines `<cs1>` to be an alias of `<cs2>`.

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, `\NewChemIUPAC` will *not* change the definition of an existing IUPAC naming command but issue an error if the IUPAC naming command already exists. `\DeclareChemIUPAC` will overwrite an existing IUPAC command.

```
1 \NewChemIUPAC\endo{\textsc{endo}}
2 \RenewChemIUPAC\anti{\textsc{anti}}
3 \iupac{(2\-\endo,7\-\anti)\-2\-\bromo\-\fluoro|bicyclo[2.2.1]heptane}
```

(2-ENDO,7-ANTI)-2-bromo-7-fluorobicyclo[2.2.1]heptane

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

```
1 \iupac{\meta{-Xylol}} \par m-Xylol
2 \RenewChemIUPAC\meta{\textup{m}} m-Xylol
3 \iupac{\meta{-Xylol}}
```

#### 5.3.4. Latin Phrases

The package `chemstyle` [Wri13] 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 `abbremp`.*

The commands are defined through

`\NewChemLatin{<cs>}{<phrase>}`

Define a new latin phrase. Gives an error if `<cs>` already exists.

`\DeclareChemLatin{<cs>}{<phrase>}`

Define a new latin phrase. Silently redefined existing macros.

`\RenewChemLatin{<cs>}{<phrase>}`

Redefine an existing latin phrase. Gives an error if `<cs>` doesn't exist.

`\ProvideChemLatin{<cs>}{<phrase>}`

Define a new latin phrase only if `<cs>` doesn't exist.

```
1 \NewChemLatin\ltn{latin text}\ltn latin text
```

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

nomenclature » `format = {⟨definition⟩}`

Default: `\itshape`

Set the format of the latin phrases.

## 5.4. The particles Module

The particles module loads the modules charges and chemformula.

### 5.4.1. Provided Particle Macros

The particles defines a number of macros which can be used for typesetting common particles in the running text. Most of them don't make much sense in chemformula [Nie15a]'s `\ch`, though, which doesn't mean that they can't be used there, of course:

`\el`  $e^-$  `\prt`  $p^+$  `\ntr`  $n^0$  `\Hyd`  $\text{OH}^-$  `\Oxo`  $\text{H}_3\text{O}^+$  `\water`  $\text{H}_2\text{O}$  `\El`  $E^+$  `\Nuc`  $\text{Nu}^-$  `\ba`  $\text{ba}^-$

All of these macros are defined using chemformula's `\chcpd`. The details are explained in section 5.4.2.

The macros `\Nuc` and `\ba` are special: they have an optional argument for the following option:

particles » `elpair = dots|dash|false`

Default: `false`

Determine how the electron pair of the nucleophiles is displayed. The electron pair is drawn using `CHEMFORMULA`'s `\chlewis` macro.

<pre>1 \ba[elpair=dots] \Nuc[elpair=dash] 2 3 \chemsetup[particles]{elpair=false} 4 \ba\ \Nuc</pre>	$\text{ba}^{\bullet-} \text{Nu}^-$ $\text{ba}^- \text{Nu}^-$
---	---

### 5.4.2. Defining Own Particle Macros

There are two sets of macros, one for defining particles and one for defining nucleophiles.

`\NewChemParticle{⟨cs⟩}{⟨formula⟩}`

Defines a new macro `⟨cs⟩`. `⟨formula⟩` is any valid `CHEMFORMULA` compound. Raises an error if `⟨cs⟩` already exists.

`\RenewChemParticle{⟨cs⟩}{⟨formula⟩}`

Redefines a new macro `⟨cs⟩`. `⟨formula⟩` is any valid `CHEMFORMULA` compound. Raises an error if `⟨cs⟩` doesn't exist.

`\DeclareChemParticle{⟨cs⟩}{⟨formula⟩}`

Defines a macro `⟨cs⟩`. `⟨formula⟩` is any valid `CHEMFORMULA` compound. Silently overwrites `⟨cs⟩` if it exists.

`\ProvideChemParticle{⟨cs⟩}{⟨formula⟩}`

Defines a new macro `⟨cs⟩`. `⟨formula⟩` is any valid `CHEMFORMULA` compound. Does nothing if `⟨cs⟩` already exists.

An example of usage is the definition of the existing particle macros:

```

1 \NewChemParticle\el {e-}
2 \NewChemParticle\prt{p+}
3 \NewChemParticle\ntn{n^0}

```

The following set defines macros like `\Nuc`

`\NewChemNucleophile{<cs>}{<formula>}`

Defines a new macro `<cs>`. `<formula>` is any valid **CHEMFORMULA** compound. Note that `<formula>` will get a trailing negative charge! Raises an error if `<cs>` already exists.

`\RenewChemNucleophile{<cs>}{<formula>}`

Redefines a new macro `<cs>`. `<formula>` is any valid **CHEMFORMULA** compound. Note that `<formula>` will get a trailing negative charge! Raises an error if `<cs>` doesn't exist.

`\DeclareChemNucleophile{<cs>}{<formula>}`

Defines a macro `<cs>`. `<formula>` is any valid **CHEMFORMULA** compound. Note that `<formula>` will get a trailing negative charge! Silently overwrites `<cs>` if it exists.

`\ProvideChemNucleophile{<cs>}{<formula>}`

Defines a new macro `<cs>`. `<formula>` is any valid **CHEMFORMULA** compound. Note that `<formula>` will get a trailing negative charge! Does nothing if `<cs>` already exists.

An example of usage is the definition of the existing nucleophile macros:

```

1 \NewChemNucleophile\Nuc{Nu}
2 \NewChemNucleophile\ba {ba}

```

A macro defined this way will have an optional argument for the `elpair` option.

## 5.5. The phases Module

The phases module loads the `chemformula` modul.

### 5.5.1. Basics

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

`\sld (s)` `\lqd (l)` `\gas (g)` `\aq (aq)`

```

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

```

---

$\text{C(s)} + 2\text{H}_2\text{O(l)} \longrightarrow \text{CO}_2\text{(g)} + 2\text{H}_2\text{(g)}$   
 To make it complete:  $\text{NaCl(aq)}$ .

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.

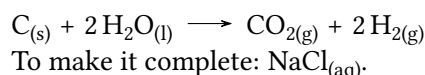
The [...] symbols are used to represent the states of aggregation of chemical species. The letters are appended to the formula in parentheses and should be printed in Roman (upright) type without a full stop (period). The IUPAC Green Book [Coh+08, p. 54]

There are two options to customize the output:

`phases` » `pos = side|sub` Default: side  
Switch the position of the phase indicator.

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

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



All those phase commands have an optional argument:

```
1 \ch{H2O "\lqd[\SI{5}{\celsius}]} H2O(l, 5 °C)
```

There is also a generic phase command:

`\phase{<phase>}`

If you need a phase indicator just once or twice. You can use it to denote a phase for which there is no phase command, yet.

### 5.5.2. Define Own Phases

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

`\NewChemPhase{<cs>}{<symbol>}`

Define a new phase command. See section 5.5.3 for a way to define language dependent settings. Gives an error if <cs> already exists.

`\DeclareChemPhase{<cs>}{<symbol>}`

Define a new phase command. See section 5.5.3 for a way to define language dependent settings. Overwrites previous definitions of <cs>.

`\RenewChemPhase{<cs>}{<symbol>}`

Redefine an existing phase command. See section 5.5.3 for a way to define language dependent settings. Gives an error if `<cs>` is not defined.

`\ProvideChemPhase{<cs>}{<symbol>}`

Define a new phase command. See section 5.5.3 for a way to define language dependent settings. Does nothing if `<cs>` is already defined.

```

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

```

---

NaOH(aq, $\infty$ ) H<sub>2</sub>O(cd) U(cr) A(lc)

NaOH<sub>(aq, $\infty$ )</sub> H<sub>2</sub>O<sub>(cd)</sub> U<sub>(cr)</sub> A<sub>(lc)</sub>

### 5.5.3. Language Dependencies

For each phase command a translation into the custom language can be defined. If a phase is declared with `\NewChemPhase` no translation exists and for every babel language the literal string is used that was provided as a definition. Let's say you define the phase

```

1 \NewChemPhase\liquid{l}

```

and want to add the German translation "fl". Then you could do

```

1 \DeclareTranslation{German}{phase-liquid}{f\l}

```

This way, when you use it in a German document using the appropriate babel option using `\liquid` would correctly translate. For this the package translations [Nie13] is used. The ID always is phase-`<csname>` where `<csname>` is the name of the phase command you defined without leading backslash.

See section 6.4 for predefined translations and general language options of `CHEMMACROS`.

## 5.6. The symbols Module

The symbols module defines a few symbols chemists need now and then. It loads the package amstext [MSoo].

`\transitionstatesymbol`

This is self-explaining:  $\neq$

`\standardstate`

Again self-explaining:  $\ominus$

`\changestate`

The uppercase delta used in  $\Delta H$  for example.

## 6. Internal Modules

### 6.1. The base Module

The base module is the core module of `CHEMMACROS`. It defines some tools which can (and should) be used in other modules. This means this section is only interesting for you if you plan to write a module yourself (see section A for details).

This module requires the packages `bm` [CMo4] and `amstext` [MSoo].

This module also provides `\chemsetup` and the option `modules`.

It also provides a number of (expl3) macros which may be used in other modules. In the macro descriptions below TF denotes that a T, an F and a TF variant exist. In case of an expandable conditional (\*) also the predicate variant is available.

\* `\chemmacros-is-int:nTF` {<number>}

Checks if <number> is an integer or not.

\* `\chemmacros-if-loaded:nnTF` {<package>|<class>}{<name>}

Checks if package (or class) <name> has been loaded. Also works after begin document.

\* `\chemmacros-if-package-loaded:nTF` {<name>}

Checks if package <name> has been loaded. Also works after begin document.

\* `\chemmacros-if-class-loaded:nTF` {<name>}

Checks if class <name> has been loaded. Also works after begin document.

`\chemmacros-leave_vmode:`

Equivalent of `\leavevmode`.

`\chemmacros-nobreak:`

Inserts a penalty of 10 000.

`\chemmacros-allow_break:`

Inserts a penalty of 0.

`\chemmacros-skip_nobreak:N` <skip/length variable>

Insert a horizontal skip while linebreak is disallowed.

`\chemmacros-if_bold:TF`

Checks if the current font weight is one of b, bc, bm, bx, bux, eb, ebc, ebx, mb, sb, sbc, sbx, ub, ubc or ubx.

`\chemmacros_bold:n` {<text>}

Checks if the current font weight is bold and if yes places <text> in `\textbf` if in text mode or in `\bm` if in math mode.

`\chemmacros_text:n {<text>}`

Ensures that *<text>* is placed in text mode.

`\chemmacros_math:n {<text>}`

Ensures that *<text>* is placed in math mode.

`\chemmacros_new_macroset:nnn {<type>} {<arg spec>} {<internal command call>}`

A command to define a set of macros `\NewChem<type>`, `\RenewChem<type>`, `\DeclareChem<type>` and `\ProvideChem<type>`. *<arg spec>* is any valid argument specification for `xparse`'s `\DeclareDocumentCommand` [L3Pb]. *<internal command call>* should be a macro which makes definitions *without* error checks, i. e., define new macros or redefine existing ones like `\def` does. This macro just should get the arguments passed on to. Have a look at the example below.

This is how the macros `\NewChemParticle`, `\RenewChemParticle`, `\DeclareChemParticle` and `\ProvideChemParticle` were defined:

```
1 \chemmacros_new_macroset:nnn {Particle} {mm}
2 { \chemmacros_define_particle:Nn #1 {#2} }
```

## 6.2. The chemformula Module

The chemformula module loads the chemformula package [Nie15a] and the amstext package [MSoo]. It also loads the charges module.

### 6.2.1. For Users

The chemformula module makes it possible that you can set all `CHEMFORMULA` options via the `\chemsetup` command using the module `chemformula`, for example:

```
1 \chemsetup[chemformula]{format=\sffamily}
```

### 6.2.2. For Module Writers

There's only one macro for module writers:

`\chemmacros_chemformula:n {<formula>}`

This is only a wrapper for `\chcpd`. It is recommended that module writers use this macro (or a variant thereof) inside of `CHEMMACROS`'s macros whenever they want to display a chemical formula. Writers who prefer traditional  $\LaTeX$  2 $\epsilon$  programming over `expl3` should use `\chcpd` directly.

## 6.3. The greek Module

The greek module loads the chemgreek package [Nie15b].

This module provides one option:



`greek = {⟨mapping⟩}`

A valid value is any valid `CHEMGREEK` `⟨mapping⟩`. `CHEMMACROS` will warn you if no mapping has been chosen or if you are using the default or the var-default mapping because this means that no upright Greek letters are available.

If you load a `CHEMGREEK` support package which allows an unambiguous choice of a mapping `CHEMGREEK` will make this choice automatically. This means if you say

```
1 \usepackage{upgreek}
2 \usepackage{chemmacros}
```

then `CHEMMACROS` will use `upgreek`'s upright Greek letters. If you have

```
1 \usepackage{upgreek}
2 \usepackage{chemmacros}
3 \usepackage{textgreek}
```

then no unambiguous choice is possible and you should choose a mapping yourself, for example:

```
1 \usepackage{upgreek}
2 \usepackage{chemmacros}
3 \usepackage{textgreek}
4 \chemsetup{greek=textgreek}
```

For further details on mappings please refer to `CHEMGREEK`'s manual.

## 6.4. The lang Module

The `lang` module provides language support for `CHEMMACROS`. It loads the package translations [Nie13].

### 6.4.1. Information For Users

This module defines the following option:

`language = auto | ⟨language⟩` Default: auto

If set to `auto` `CHEMMACROS` will detect the language used by `babel` [Bra13] or `polyglossia` [Cha13] automatically, fallback is English. Any language known to the translations package is a valid value for `⟨language⟩`.

The language chosen via `language` is used for translation of certain strings in different places all over `CHEMMACROS`. They are mentioned in the places when the corresponding function of `CHEMMACROS` is explained.

Translation is done with the help of the translations package, available translation keys are listed in section 6.4.2.

TABLE 3: Translation keys predefined by **CHEMMACROS**.

key	fallback translation	German
scheme-name	Scheme	Schema
scheme-list	List of Schemes	Verzeichnis der Schemata
K-acid	$\mathrm{a}$	$\mathrm{s}$
K-base	$\mathrm{b}$	
K-water	$\mathrm{w}$	
phase-sld	s	f
phase-lqd	l	f\l
phase-gas	g	
phase-aq	aq	
list-of-reactions	List of Reactions	Reaktionsverzeichnis
reaction	Reaction	Reaktion

#### 6.4.2. Available Translation Keys

Table 3 lists (almost) all keys which are predefined in **CHEMMACROS**. A translation key is a key which is understood by the translations package and its commands like `\GetTranslation`. For each key at least the English fallback translation is provided, for most also the German translation is provided. For a few keys also other translations are provided. If you find that your translation is missing you can provide it in the preamble:

`\DeclareTranslation{<language>}{<key>}{<translation>}`

Defines a translation of key `<key>` for the language `<language>`. No error will be raised if a translation of `<key>` already exists. This command can only be used in the preamble and is defined by the translations package.

If you send me an email (see section B on page 58) with the translations for your language I'll gladly add them to the next release of **CHEMMACROS**!

#### 6.4.3. Information For Module Writers

\* `\chemmacros_translate:n {<translation key>}`

Translates the given key to the language which is detected automatically or given by the user. Should be used in **CHEMMACROS**'s macros instead of translations' `\GetTranslation`.

`\l_chemmacros_language_tl`

A token list variable that holds the language which is used by `\chemmacros_translate:n` for translation, *after begin document*.

`\ChemTranslate{<translation key>}`

A version of `\chemmacros_translate:n` for those who prefer traditional  $\text{\LaTeX 2}_{\epsilon}$  programming over `expl3`.

## Part III.

# Additional Modules

### 7. User Modules

#### 7.1. The all pseudo-module

The all module is a pseudo module: it doesn't define any functionality at all. It does however load all other modules. So you can say

```
1 \chemsetup{ modules = all }
```

to ensure that every module is available. This *will not* load personal modules!

#### 7.2. The isotopes Module

The isotope module loads the elements package [Nie15c]. This module defines one user command:

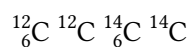
`\isotope*{⟨input⟩}`

⟨input⟩ can either be the *symbol* of an element or the *name* of an element. Be aware that *the name is language dependent*, refer to the manual of the elements package for details. To be on the safe side use the element symbol.

⟨input⟩ can also be comma separated list: `\isotope{⟨nuc⟩,⟨symbol⟩}`. If you leave ⟨nuc⟩ out then `\isotope` will display the most common isotope. Otherwise ⟨nuc⟩ will be used. If ⟨nuc⟩ is an isotope unknown to the elements package `\isotope` will write a warning to the log file.

The starred variant omits the element number.

```
1 \isotope{C}
2 \isotope*{C}
3 \isotope{14,C}
4 \isotope*{14,C}
```



As input for the element symbol you can choose any of the elements known to the elements package.

There are options which allow you to determine how the isotope is printed:

`isotopes » format = super|side` Default: super  
Either print the isotope number as superscript or to the right of the element symbol.

`isotopes » side-connect = {⟨input⟩}` Default: -  
Determine what is printed between the element symbol and the isotope number if `format = {side}`.

```

1 \isotope{C}
2 \chemsetup[isotopes]{format=side}
3 \isotope{C}
4 \chemsetup[isotopes]{side-connect=}
5 \isotope{C}

```

$$^{12}_6\text{C} \quad \text{C-12} \quad \text{C}_{12}$$

### 7.3. The mechanisms Module

The module mechanisms loads the package amstext [MSoo]. It provides one macro:

`\mech[⟨type⟩]`

Allows to specify the most common reaction mechanisms.

⟨type⟩ can have one of the following values:

`\mech`

(empty, no opt. argument) nucleophilic substitution S<sub>N</sub>

`\mech[1]`

unimolecular nucleophilic substitution S<sub>N</sub>1

`\mech[2]`

bimolecular nucleophilic substitution S<sub>N</sub>2

`\mech[se]`

electrophilic substitution S<sub>E</sub>

`\mech[1e]`

unimolecular electrophilic substitution S<sub>E</sub>1

`\mech[2e]`

bimolecular electrophilic substitution S<sub>E</sub>2

`\mech[ar]`

electrophilic aromatic substitution Ar-S<sub>E</sub>

`\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<sub>cb</sub>

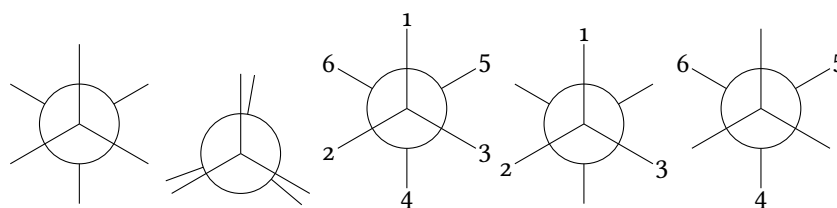
### 7.4. The newman Module

The newman module provides a command for drawing Newman projections. It loads the tikz module.

`\newman[⟨options⟩](⟨angle⟩){⟨1⟩,⟨2⟩,⟨3⟩,⟨4⟩,⟨5⟩,⟨6⟩}`

Create Newman projections. This command uses TikZ internally.  $\langle angle \rangle$  rotates the back atoms counter clockwise with respect to the front atoms and is an optional argument.  $\langle 1 \rangle$  to  $\langle 6 \rangle$  are the positions, the first three are the front atoms, the last three the back atoms.

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

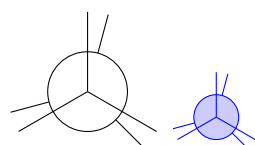


Several options allow customization:

- |  |                   |
|--|-------------------|
| <code>newman</code> » <code>angle = {⟨angle⟩}</code>               | Default: 0        |
| Default angle.   |                   |
| <code>newman</code> » <code>scale = {⟨factor⟩}</code>              | Default: 1        |
| Scale the whole projection by factor $\langle factor \rangle$ .    |                   |
| <code>newman</code> » <code>ring = {⟨tikz⟩}</code>                 | (initially empty) |
| Customize the ring with TikZ keys.                                 |                   |
| <code>newman</code> » <code>atoms = {⟨tikz⟩}</code>                | (initially empty) |
| Customize the nodes within which the atoms are set with TikZ keys. |                   |
| <code>newman</code> » <code>back-atoms = {⟨tikz⟩}</code>           | (initially empty) |
| Explicitly customize the nodes of the back atoms with TikZ keys.   |                   |

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

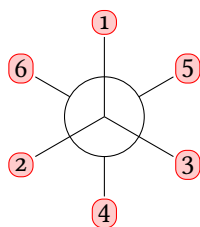
```



```

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

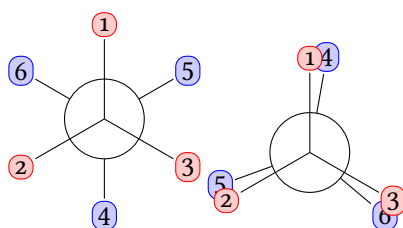
```



```

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

```



### 7.5. The orbital Module

The orbital module loads the tikz module. It provides the following command to create orbitals:

`\orbital[⟨options⟩]{⟨type⟩}`

Draw an orbital shape of type *⟨type⟩*. This command uses TikZ internally.

There are the following types available for *⟨type⟩*:

s   p   sp   sp2   sp3

```

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

```



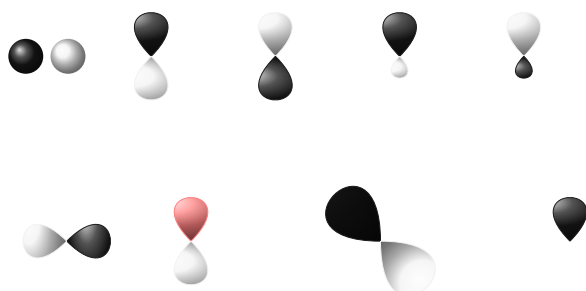
Depending on the type you have different options to modify the orbitals:

<code>orbital</code> » <code>phase = + -</code>	Default: +
changes the phase of the orbital (all types)	
<code>orbital</code> » <code>scale = {⟨factor⟩}</code>	Default: 1
changes the size of the orbital (all types)	
<code>orbital</code> » <code>color = {⟨color⟩}</code>	Default: black
changes the color of the orbital (all types)	
<code>orbital</code> » <code>angle = {⟨angle⟩}</code>	Default: 0
rotates the orbitals with a p contribution counter clockwise (all types except s)	
<code>orbital</code> » <code>half = true false</code>	Default: false
displays only half an orbital (only p)	

```

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

```



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

`orbital` » `overlay = true|false`

The orbital “doesn’t need space”; it is displayed with the TikZ option `overlay`.

`orbital` » `opacity = {⟨num⟩}`

The orbital becomes transparent; `⟨value⟩` can have values between 1 (fully opaque) to 0 (invisible).

```

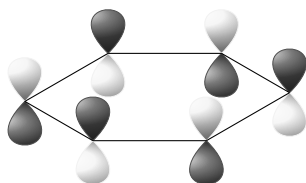
1 \vspace{7mm}
2 \chemsetup[orbital]{
3   overlay,
4   p/color = black!70
5 }

```

```

6 \setbondoffset{0pt}
7 \chemfig{
8   ?\orbital{p}
9   -[,1.3]{\orbital[phase=-]{p}}
10  -[:30,1.1]\orbital{p}
11  -[:150,.9]{\orbital[phase=-]{p}}
12  -[4,1.3]\orbital{p}
13  -[: -150,1.1]{\orbital[phase=-]{p}}?
14 }
15 \vspace{7mm}

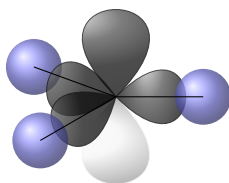
```



```

1 \vspace{7mm}
2 \setbondoffset{0pt}
3 \chemsetup[orbital]{
4   overlay ,
5   opacity = .75 ,
6   p/scale = 1.6 ,
7   s/color = blue!50 ,
8   s/scale = 1.6
9 }
10 \chemfig{
11   \orbital{s}
12   -[: -20]{\orbital[scale=2]{p}}
13           {\orbital[half,angle=0]{p}}
14           {\orbital[angle=170,half]{p}}
15           {\orbital[angle=-150,half]{p}}
16   (-[: -150]\orbital{s})-\orbital{s}
17 }
18 \vspace{1cm}

```



## 7.6. The reactions Module

The reactions module loads the chemformula module and the mathtools package [MRW13].



## 7.6.1. Predefined Environments

You can use these environments for numbered...

`\begin{reaction}`

A single reaction where `CHEMFORMULA` code is placed directly in the environment body. A wrapper around the equation environment.

`\begin{reactions}`

Several aligned reactions. A wrapper around amsmath's align environment.

...and their starred versions for unnumbered reactions.

`\begin{reaction*}`

A wrapper around the equation\* environment.

`\begin{reactions*}`

A wrapper around amsmath's align\* environment.

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

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

```
1 Reaction with counter:
2 \begin{reaction}
3   A -> B
4 \end{reaction}
```

---

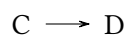
Reaction with counter:



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

---

Reaction without counter:



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

Several aligned reactions with counter:

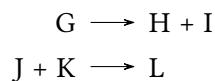


```

1 Several aligned reactions without counter:
2 \begin{reactions*}
3   G      &-> H + I \\
4   J + K &-> L
5 \end{reactions*}

```

Several aligned reactions without counter:



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

`\renewtagform{<tagname>}[<format>]{<right delimiter>}{<left delimiter>}`  
 Provided by the mathtools package.

```

1 \renewtagform{reaction}[R \textbf{}]{[]{}]}
2 \begin{reaction}
3   H2O + CO2 <=> H2CO3
4 \end{reaction}

```



The use of  $\mathcal{A}\mathcal{M}\mathcal{S}\text{math}$ 's `\intertext` is possible:

```

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

```



Some text in between aligned reactions



See reaction 5.

### 7.6.2. Own Reactions

You can create new types of reactions with the command:

`\NewChemReaction{<name>}[<number of arguments>]{<math name>}`

`<name>` will be the name of the new chem environment. `<math name>` is the underlying math environment. Gives an error if `<name>` already exists.

`\RenewChemReaction{<name>}[<number of arguments>]{<math name>}`

`<name>` is the name of the renewed chem environment. `<math name>` is the underlying math environment. Gives an error if `<name>` does not exist.

`\DeclareChemReaction{<name>}[<number of arguments>]{<math name>}`

`<name>` will be the name of the chem environment. `<math name>` is the underlying math environment.

`\ProvideChemReaction{<name>}[<number of arguments>]{<math name>}`

`<name>` will be the name of the new chem environment. `<math name>` is the underlying math environment. The new environment is only defined if it doesn't exist, yet.

```
1 \NewChemReaction{reaction} {equation}
2 \NewChemReaction{reaction*} {equation*}
3 \NewChemReaction{reactions} {align}
4 \NewChemReaction{reactions*}{align*}
```

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

```
1 \NewChemReaction{reactionsat}[1]{alignat}
```

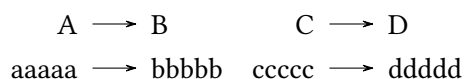
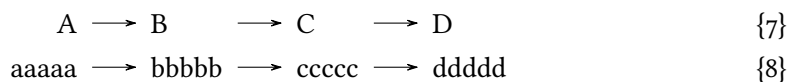
With this the reactionsat environment is defined.

```
1 \NewChemReaction{reactionsat}[1]{alignat}
2 \NewChemReaction{reactionsat*}[1]{alignat*}
3 \begin{reactionsat}{3}
```

```

4   A      &-> B      &&-> C      &&-> D  \
5   aaaaa &-> bbbbb &&-> ccccc &&-> ddddd
6   \end{reactionsat}
7   \begin{reactionsat*}{2}
8   A      &-> B      & C              &-> D  \
9   aaaaa &-> bbbbb &\quad{} ccccc &-> ddddd
10  \end{reactionsat*}

```



### 7.6.3. List of Reactions

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

`\listoreactions`

Print a list of reactions.

```

1 \listoreactions

```

### List of Reactions

Reaction {1} . . . . .	33
Reaction {2} . . . . .	34
Reaction {3} . . . . .	34
Reaction [R 4] . . . . .	34
Reaction {5} . . . . .	35
Reaction {6} . . . . .	35
Reaction {7} . . . . .	36
Reaction {8} . . . . .	36
Reaction {9}: Autoprotolyse . . . . .	37
Reaction {10}: first step of chain . . . . .	37
Reaction {11}: second step of chain . . . . .	37

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

`reaction » list-name = {⟨name of the list⟩}` Default: List of reactions  
 Let's you set the name of the list manually. The default name is language dependent, see section 6.4.

`reaction » list-entry = {⟨prefix to each entry⟩}` Default: Reaction  
 Let's you set a prefix to each list entry. The default name is language dependent, see section 6.4.

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

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

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

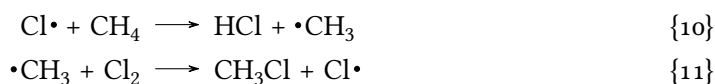


If you use the reactions environment this will not work, though. In this case you can use

`\AddRxnDesc{⟨description⟩}`

Add a description to a reaction.

```
1 \begin{reactions}
2   "\chlewis{0.}{Cl}" + CH4 &
3   -> HCl + "\chlewis{180.}{C}" H3 \AddRxnDesc{first-step-of-chain} \
4   "\chlewis{180.}{C}" H3 + Cl2 &
5   -> CH3Cl + "\chlewis{0.}{Cl}" \AddRxnDesc{second-step-of-chain}
6 \end{reactions}
```



## 7.7. The redox Module

The redox module loads the modules `tikz` and `xfrac`. It also loads the packages `math-tools` [MRW13] and `relsize` [Ars13].

### 7.7.1. Oxidation Numbers

Regarding the typesetting of oxidation numbers *The IUPAC Green Book* [Coh+08] says the following:

## 7. User Modules

Oxidation numbers are denoted by positive or negative Roman numerals or by zero [...]

Examples  $\text{Mn}^{\text{VII}}$ , manganese (VII),  $\text{O}^{-\text{II}}$ ,  $\text{Ni}^0$  [Coh+08, p. 50]

The following command is provided to set oxidation numbers:

`\ox*[\langle options \rangle]{\langle number \rangle,\langle atom \rangle}`

Places  $\langle number \rangle$  as right superscript to  $\langle atom \rangle$ ;  $\langle number \rangle$  has to be a (rational) number!  $\langle atom \rangle$  is treated as a **CHEMFORMULA** formula, like it would be in `\chcpd`.

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

$\text{Na}^{\text{I}}$ ,  $\text{Ca}^{\text{II}}$ ,  $\text{S}^{-\text{II}}$ ,  $\text{F}^{-\text{I}}$

There are a number of options that can be used to modify the typeset result:

`redox » parse = true|false` Default: true  
When false an arbitrary entry can be used for  $\langle number \rangle$ .

`redox » roman = true|false` Default: false  
Switches from roman to arabic numbers.

`redox » pos = top|super|side` Default: super  
top places  $\langle number \rangle$  above  $\langle atom \rangle$ , super to the upper right as superscript and side to the right and inside brackets. Both super and side follow IUPAC recommendation, top does not!

`redox » explicit-sign = true|false` Default: false  
Shows the + for positiv numbers and the  $\pm$  for 0.

`redox » decimal-marker = comma|point` Default: point  
Choice for the decimal marker for formal oxidation numbers like  $\text{X}^{1.2}$ .

`redox » align = center|right` Default: center  
Center the oxidation number relative to the atom or right-align it.

`redox » side-connect = {\langle code \rangle}` Default: `\,`  
Code that is inserted between atom and oxidation number if `pos = {side}` is used.

`redox » text-fraction = {\langle cs \rangle}` Default: `\chemfrac[text]{#1}{#2}`  
The fraction macro that is used for fractions if `pos = {side}` is used.  $\langle cs \rangle$  must be a macro that takes two mandatory arguments, the first for the numerator and the second for the denominator.

`redox » super-fraction = {\langle cs \rangle}` Default: `\chemfrac[superscript]{#1}{#2}`  
The fraction macro that is used for fractions if `pos = {top}` or `pos = {super}` is used.  $\langle cs \rangle$  must be a macro that takes two mandatory arguments, the first for the numerator and the second for the denominator.

## 7. User Modules

```

1 \ox[roman=false]{2,Ca} \ox{2,Ca} \
2 \ox[pos=top]{3,Fe}-Oxide \
3 \ox[pos=side]{3,Fe}-Oxide \
4 \ox[parse=false]{?,Mn} \
5 \ox[pos=top,align=right]{2,Ca}

```

$$\text{Ca}^2 \text{Ca}^{\text{II}}$$

$$\text{Fe}^{\text{III}}\text{-Oxide}$$

$$\text{Fe (III)-Oxide}$$

$$\text{Mn}^?$$

$$\text{Ca}^{\text{II}}$$

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

```

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

```

$$\text{Fe}^{\text{III}} \text{Fe}^{\text{III}}$$

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

```

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

```

---


$$\text{Na}^{+1}, \text{Ca}^{+2}, \text{S}^{-2}, \text{F}^{\pm 0}_2$$

```

1 \chemsetup[redox]{pos=top}
2 Compare \ox{-1,O2^2-} to \ch{"\ox{-1,O}" {}2^2-}

```

---


$$\text{Compare } \text{O}_2^{-1 2-} \text{ to } \text{O}_2^{-1 2-}$$

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

```

1 \chemsetup[redox]{pos=top}
2 \ox{.5,Br2}
3 \ch{"\ox{1/3,I}" {}3+}
4
5 \chemsetup[redox]{pos=side}
6 \ox{1/3,I3+}

```

$$\text{Br}_2 \text{I}_3^{+0.5 \frac{1}{3}}$$

$$\text{I}_3^{+} (\frac{1}{3})$$

The fraction is displayed with the help of the `xfrac` package [L3Pb]. For more details on how **CHEMMACROS** uses it read section 8.2.

### 7.7.2. Redox Reactions

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

`\OX{⟨name⟩,⟨atom⟩}`

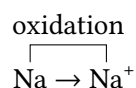
Label  $\langle atom \rangle$  with the label  $\langle name \rangle$ .

`\redox(⟨name1⟩,⟨name2⟩)[⟨tikz⟩][⟨num⟩]{⟨text⟩}`

Connect two  $\langle atom \rangle$ s previously labelled with `\OX`. Only the first argument ( $\langle name1 \rangle, \langle name2 \rangle$ ) is required, the others are all optional.

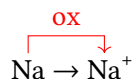
`\OX` places  $\langle atom \rangle$  into a node, which is named with  $\langle name \rangle$ . If you have set two `\OX`, they can be connected with a line using `\redox`. To do so the names of the two nodes that are to be connected are written in the round braces. Since `\redox` draws a `tikzpicture`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

```
1 \vspace{7mm}
2 \OX{a,Na} $\rightarrow$ \OX{b,Na}\pch\redox(a,b){oxidation}
```



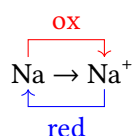
This line can be customized using TikZ keys in `[⟨tikz⟩]`:

```
1 \vspace{7mm}
2 \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  $\langle num \rangle$ . If you use a negative value the line is placed *below* the text.

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





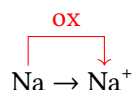
The default length of the vertical lines can be customized with the option

`redox » dist = {<dim>}`

Default: .6em

A TeX dimension.

```
1 \vspace{7mm}
2 \chemsetup{redox/dist=1em}
3 \OX{a,Na} $\rightarrow$ \OX{b,Na}\pch\redox(a,b)[->,red]{ox}
```

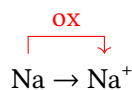


`redox » sep = {<dim>}`

Default: .2em

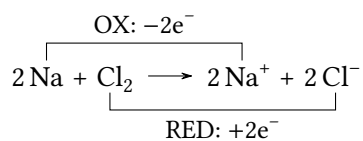
The option can be used to change the distance between the atom and the beginning of the line.

```
1 \vspace{7mm}
2 \chemsetup{redox/sep=.5em}
3 \OX{a,Na} $\rightarrow$ \OX{b,Na}\pch\redox(a,b)[->,red]{ox}
```



## Examples

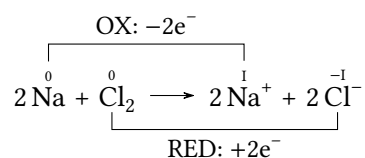
```
1 \vspace{7mm}
2 \ch{
3   2 "\OX{o1,Na}" + "\OX{r1,Cl}" {}2
4   ->
5   2 "\OX{o2,Na}" {}+ + 2 "\OX{r2,Cl}" {}-
6 }
7 \redox(o1,o2){\small OX: $- 2\text{e}^-$}
8 \redox(r1,r2){}[-1]{\small RED: $+ 2\text{e}^-$}
9 \vspace{7mm}
```



```

1 \vspace{7mm}
2 \ch{
3   2 "\OX{o1,\ox*{0,Na}}" + "\OX{r1,\ox*{0,Cl}}" {}2
4   ->
5   2 "\OX{o2,\ox*{+1,Na}}" {}+ + 2 "\OX{r2,\ox*{-1,Cl}}" {}-
6 }
7 \redox(o1,o2){\small OX: $- 2\el$}
8 \redox(r1,r2){\small RED: $+ 2\el$}
9 \vspace{7mm}

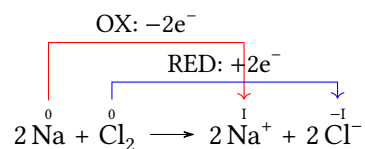
```



```

1 \vspace{14mm}
2 \ch{
3   2 "\OX{o1,\ox*{0,Na}}" + "\OX{r1,\ox*{0,Cl}}" {}2
4   ->
5   2 "\OX{o2,\ox*{+1,Na}}" {}+ + 2 "\OX{r2,\ox*{-1,Cl}}" {}-
6 }
7 \redox(o1,o2)[draw=red,->][3.33]{\small OX: $- 2\el$}
8 \redox(r1,r2)[draw=blue,->]{\small RED: $+ 2\el$}

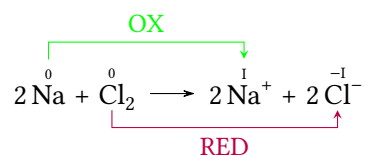
```



```

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

```



## 7.8. The scheme Module

The scheme module defines a floating environment `\begin{scheme}`. That is, it *only* defines this float if no environment scheme exists at begin document. The module checks for different available float defining methods, in *this* order:

- If the current class is a KOMA-Script class `\DeclareNewTOC` will be used.
- If the current class is memoir, memoir's methods are used.
- If the package tocbasic has been loaded `\DeclareNewTOC` will be used.
- If the package newfloat has been loaded `\DeclareFloatingEnvironment` will be used.
- If the package float has been loaded its method will be used.
- If neither of the above the “manual” method is used. This means the environment is defined the same way like figure is defined in the article class or the book class, depending if `\chapter` is defined or not.

The list name and the caption name both are translated to the language specified according to the `lang` option and the provided translations, see section 6.4 for details. If you want to manually change them then redefine these macros after begin document:

`\listscasename`

The name of the list of schemes.

`\schemename`

The name used in captions.

The list of schemes is printed as expected with

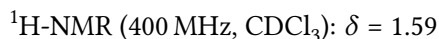
`\listofschemes`

## 7.9. The spectroscopy Module

The spectroscopy module loads the chemformula module and the siunitx package [Wri15].

### 7.9.1. 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:



The spectroscopy module provides a command which simplifies the input.

`\NMR*{<num>,<element>}(<num>,<unit>)[<solvent>]`

Typeset nuclear magnetic resonance data. `<num>` is a valid siunitx number input, `<unit>` is a valid siunitx unit input. `<solvent>` is any valid `CHEMFORMULA` input as in `\chcpd`.

*All Argument are optional! Without arguments we get:*

1	<code>\NMR \par</code>	$^1\text{H-NMR: } \delta$
2	<code>\NMR*</code>	$^1\text{H-NMR}$

The first argument specifies the kind of NMR:

1	<code>\NMR{13,C}</code>	$^{13}\text{C-NMR: } \delta$
---	-------------------------	------------------------------

The second argument sets the frequency (in MHz):

1	<code>\NMR(400)</code>	$^1\text{H-NMR (400 MHz): } \delta$
---	------------------------	-------------------------------------

You can choose another unit:

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

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

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

The third argument specifies the solvent:

1	<code>\NMR[CDCl3]</code>	$^1\text{H-NMR (CDCl}_3\text{): } \delta$
---	--------------------------	---

### 7.9.2. Short Cuts

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

`\NewChemNMR{<cs>}{<num>,<atom>}`

Define a new shortcut macro for typesetting a certain type of magnetic resonance data. Gives an error if <cs> already exists.

`\DeclareChemNMR{<cs>}{<num>,<atom>}`

Define a new shortcut macro for typesetting a certain type of magnetic resonance data. Overwrites an existing macro.

`\RenewChemNMR{<cs>}{<num>,<atom>}`

Redefine an existing shortcut macro for typesetting a certain type of magnetic resonance data. Gives an error if <cs> doesn't exist.

`\ProvideChemNMR{<cs>}{<num>,<atom>}`

Define a new shortcut macro for typesetting a certain type of magnetic resonance data. <cs> is only defined if it doesn't exist, yet.

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

1 <code>\NewChemNMR\HNMR{1,H}%</code>	$^{13}\text{C}$ -NMR (100 MHz)
2 <code>\NewChemNMR\CNMR{13,C}%</code>	
3 <code>\CNMR*(100) \par</code>	$^1\text{H}$ -NMR (400 MHz)
4 <code>\HNMR*(400)</code>	

### 7.9.3. An Environment to Typeset Experimental Data

The spectroscopy module provides an environment to ease the input of experimental data.

`\begin{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]}`  $^{13}\text{C}\{^1\text{H}\}$ -NMR:  $\delta$

`\J(<bonds>;<nuclei>)[<unit>]{<list of nums>}`

Coupling constant, values are input separated by ; (NMR). The arguments (<bonds>;<nuclei>) and [<unit>] are optional and enable further specifications of the coupling.

`\#{<num>}`

Number of nuclei (NMR).

`\pos{<num>}`

Position of nuclues (NMR).

`\val{<num>}`

A number, an alias of siunitx' `\num{<num>}`.

`\val{<num1>-<num2>}`

An alias of siunitx' `\numrange{<num1>}{<num2>}`.

```

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

```

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

**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`.

- `spectroscopy` » `unit = {⟨unit⟩}` Default: `\mega\hertz`  
The used default unit.
- `spectroscopy` » `nucleus = {⟨num⟩,⟨atom⟩}` Default: `{1,H}`  
The used default nucleus.
- `spectroscopy` » `connector = {⟨code⟩}` Default: `-`  
Places `⟨code⟩` between the nucleus and the method.
- `spectroscopy` » `method = {⟨code⟩}` Default: `NMR`  
The measuring method.
- `spectroscopy` » `format = {⟨commands⟩}` (initially empty)  
For example `\bfseries`.
- `spectroscopy` » `pos-number = side|sub|super` Default: `side`  
Position of the number next to the atom.
- `spectroscopy` » `coupling-symbol = {⟨code⟩}` Default: `J`  
The symbol used for the coupling constant.
- `spectroscopy` » `coupling-unit = {⟨unit⟩}` Default: `\hertz`  
A siunitx unit.
- `spectroscopy` » `coupling-pos = side|sub` Default: `side`  
Placement of the coupling nuclei next to the symbol `J` (or rather the symbol specified with option `coupling-symbol`).
- `spectroscopy` » `coupling-nuclei-pre = {⟨code⟩}` Default: `(`  
Code inserted before the coupling nuclei when `coupling-pos = {side}`.
- `spectroscopy` » `coupling-nuclei-post = {⟨code⟩}` Default: `)`  
Code inserted after the coupling nuclei when `coupling-pos = {side}`.
- `spectroscopy` » `coupling-bonds-pre = {⟨code⟩}` (initially empty)  
Code inserted before the coupling bonds.
- `spectroscopy` » `coupling-bonds-post = {⟨code⟩}` Default: `\!`  
Code inserted after the coupling bonds.
- `spectroscopy` » `coupling-pos-cs = {⟨cs⟩}` Default: `\@firstofone`  
Set the macro that prints the number set with the `\pos` macro. This needs to be a command with one mandatory argument.
- `spectroscopy` » `atom-number-cs = {⟨cs⟩}` Default: `\@firstofone`  
Set the macro that prints the number set with the `\#` macro. This needs to be a command with one mandatory argument.
- `spectroscopy` » `parse = true|false` Default: `true`  
Treat the solvent as `CHEMFORMULA` formula or not.

spectroscopy » `delta = {⟨tokens⟩}` (initially empty)  
 The `⟨tokens⟩` are added after `δ`.

spectroscopy » `list = true|false` Default: false  
 The environment nmr is formatted as a list

spectroscopy » `list-setup = {⟨setup⟩}`  
 Setup of the list. See below for the default settings.

spectroscopy » `use-equal = true|false` Default: false  
 Add equal sign after `\NMR` and `\data`.  
 The default setup of the list:

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

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

---

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

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

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

---

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

**An Example** The code below is shown with different specifications for `⟨options⟩`. Of course options can also be chosen with `\chemsetup`.

## 7. User Modules

```

1 \sisetup{separate-uncertainty,per-mode=symbol,detect-all,range-phrase=- -}
2 \begin{experimental}[<optionen>]
3   \data*{yield} \SI{17}{\milli\gram} yellow needles (\SI{0.04}{\milli\mole},
4     \SI{13}{\percent}).
5   %
6   \data{mp.} \SI{277}{\celsius} (DSC).
7   %
8   \NMR{600}[CDCl3] \val{2.01} (s, \#{24}, \pos{5}), \val{2.31} (s, \#{12},
9     \pos{1}), \val{6.72--6.74} (m, \#{2}, \pos{11}), \val{6.82} (s, \#{8},
10    \pos{3}), \val{7.05--7.07} (m, \#{2}, \pos{12}), \val{7.39--7.41} (m, \#{4},
11    \pos{9}), \val{7.48--7.49} (m, \#{4}, \pos{8}).
12   %
13   \NMR{13,C}(150)[CDCl3] \val{21.2} ($+$, \#{4}, \pos{1}), \val{23.4} ($+$,
14     \#{8}, \pos{5}), \val{126.0} ($+$, \#{4}, \pos{9}), \val{128.2} ($+$, \#{8},
15     \pos{3}), \val{130.8} ($+$, \#{2}, \pos{12}), \val{133.6} ($+$, \#{2},
16     \pos{11}), \val{137.0} ($+$, \#{4}, \pos{8}), \val{138.6} (q, \#{4},
17     \pos{2}), \val{140.6} (q, \#{2}, \pos{10}), \val{140.8} (q, \#{8}, \pos{4}),
18     \val{141.8} (q, \#{4}, \pos{6}), \val{145.6} (q, \#{2}, \pos{7}).
19   %
20   \data{MS}[DCP, EI, \SI{60}{\electronvolt}] \val{703} (2, \ch{M+}), \val{582}
21     (1), \val{462} (1), \val{249} (13), \val{120} (41), \val{105} (100).
22   %
23   \data{MS}[\ch{MeOH + H2O + KI}, ESI, \SI{10}{\electronvolt}] \val{720} (100,
24     \ch{M+ + OH-}), \val{368} (\ch{M+ + 2 OH-}).
25   %
26   \data{IR}[KBr] \val{3443} (w), \val{3061} (w), \val{2957} (m), \val{2918}
27     (m), \val{2856} (w), \val{2729} (w), \val{1725} (w), \val{1606} (s),
28     \val{1592} (s), \val{1545} (w), \val{1446} (m), \val{1421} (m), \val{1402}
29     (m), \val{1357} (w), \val{1278} (w), \val{1238} (s), \val{1214} (s),
30     \val{1172} (s), \val{1154} (m), \val{1101} (w), \val{1030} (w), \val{979}
31     (m), \val{874} (m), \val{846} (s), \val{818} (w), \val{798} (m), \val{744}
32     (w), \val{724} (m), \val{663} (w), \val{586} (w), \val{562} (w), \val{515}
33     (w).
34   %
35   \data*{UV-Vis} \SI{386}{\nano\metre} ($\varepsilon = \val{65984}$),
36     \SI{406}{\nano\metre} ($\varepsilon = \val{65378}$).
37   %
38   \data*{quantum yield} $\Phi = \val{0.74+-0.1}$\%,.
39 \end{experimental}

```

**Nearly Standard** Output with these options:

```

1 delta=(ppm),pos-number=sub,use-equal

```

yield: 17 mg yellow needles (0.04 mmol, 13 %). mp. = 277 °C (DSC). <sup>1</sup>H-NMR (600 MHz, CDCl<sub>3</sub>): δ (ppm) = 2.01 (s, 24 H, H<sub>5</sub>), 2.31 (s, 12 H, H<sub>1</sub>), 6.72–6.74 (m, 2 H, H<sub>11</sub>), 6.82 (s, 8 H, H<sub>3</sub>), 7.05–7.07 (m, 2 H, H<sub>12</sub>), 7.39–7.41 (m, 4 H, H<sub>9</sub>), 7.48–7.49 (m, 4 H, H<sub>8</sub>). <sup>13</sup>C-NMR (150 MHz, CDCl<sub>3</sub>): δ (ppm) = 21.2 (+, 4 C, C<sub>1</sub>), 23.4 (+, 8 C, C<sub>5</sub>), 126.0 (+, 4 C, C<sub>9</sub>), 128.2 (+, 8 C, C<sub>3</sub>), 130.8 (+, 2 C, C<sub>12</sub>), 133.6 (+, 2 C, C<sub>11</sub>), 137.0 (+, 4 C, C<sub>8</sub>), 138.6 (q, 4 C, C<sub>2</sub>), 140.6 (q, 2 C, C<sub>10</sub>), 140.8 (q, 8 C, C<sub>4</sub>), 141.8 (q, 4 C,



C<sub>6</sub>), 145.6 (q, 2 C, C<sub>7</sub>). MS (DCP, EI, 60 eV) = 703 (2, M<sup>+</sup>), 582 (1), 462 (1), 249 (13), 120 (41), 105 (100). MS (MeOH + H<sub>2</sub>O + KI, ESI, 10 eV) = 720 (100, M<sup>+</sup> + OH<sup>-</sup>), 368 (M<sup>+</sup> + 2 OH<sup>-</sup>). IR (KBr) = 3443 (w), 3061 (w), 2957 (m), 2918 (m), 2856 (w), 2729 (w), 1725 (w), 1606 (s), 1592 (s), 1545 (w), 1446 (m), 1421 (m), 1402 (m), 1357 (w), 1278 (w), 1238 (s), 1214 (s), 1172 (s), 1154 (m), 1101 (w), 1030 (w), 979 (m), 874 (m), 846 (s), 818 (w), 798 (m), 744 (w), 724 (m), 663 (w), 586 (w), 562 (w), 515 (w). UV-Vis: 386 nm ( $\epsilon$  = 65 984), 406 nm ( $\epsilon$  = 65 378). quantum yield:  $\Phi$  = 0.74 ± 0.10.

**Formatted List** Output with these options:

```
1 format=\bfseries,delta=(ppm),list=true,use-equal
```

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

**mp.** = 277 °C (DSC).

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

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

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

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

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

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

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

**Crazy** Output for these options:

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

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

**mp.** = 277 °C (DSC).

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

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

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

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

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

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

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

### 7.10. The thermodynamics Module

The thermodynamics module loads the siunitx package [Wri15].

#### 7.10.1. The `\state` Macro

`\state[options]{symbol}`

Typeset a state variable.

This macro can be used to write the thermodynamic state variables.

```
1 \state{A}, \state[subscript-left=f]{G} ,
2 \state[subscript-right=ch{Na}]{E},
3 \state[superscript-right=SI{1000}]{celsius}{H}
```

---

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

These options are available:

`thermodynamics` » `pre` = { $\langle text \rangle$ }

Default: `\changestate`

The symbol before the variable. Inserted in text mode.

`thermodynamics` » `superscript-left` = { $\langle text \rangle$ }

(initially empty)

The left superscript. Inserted in text mode.

`thermodynamics` » `superscript-right` = { $\langle text \rangle$ }

Default: `\standardstate`

The right superscript. Inserted in text mode.

`thermodynamics` » `superscript` = { $\langle text \rangle$ }

An alias of `superscript-right`.

`thermodynamics` » `subscript-left` = { $\langle text \rangle$ }

(initially empty)

The left subscript. Inserted in text mode.

`thermodynamics` » `subscript-right` =  $\{\langle text \rangle\}$  (initially empty)  
 The right subscript. Inserted in text mode.

`thermodynamics` » `subscript` =  $\{\langle text \rangle\}$   
 An alias of `subscript-left`.

### 7.10.2. Thermodynamic Variables

The thermodynamics module provides a few commands for specific thermodynamic variables:

`\enthalpy*`[ $\langle options \rangle$ ]( $\langle subscript \rangle$ ){ $\langle value \rangle$ }  
 Typeset the amount of enthalpy.

`\entropy*`[ $\langle options \rangle$ ]( $\langle subscript \rangle$ ){ $\langle value \rangle$ }  
 Typeset the amount of entropy.

`\gibbs*`[ $\langle options \rangle$ ]( $\langle subscript \rangle$ ){ $\langle value \rangle$ }  
 Typeset the amount of Gibbs enthalpy.

Their usage is pretty much self-explaining:

<code>1 \enthalpy{123} \par</code> <code>2 \entropy{123} \par</code> <code>3 \gibbs{123}</code>	$\Delta H^\circ = 123 \text{ kJ mol}^{-1}$ $S^\circ = 123 \text{ J K}^{-1} \text{ mol}^{-1}$ $\Delta G^\circ = 123 \text{ kJ mol}^{-1}$
---	---

The argument ( $\langle subscript \rangle$ ) adds a subscript for specification, \* hides number and unit:

<code>1 \enthalpy(r){123} \par</code> <code>2 \enthalpy*{123} \par</code>	$\Delta_r H^\circ = 123 \text{ kJ mol}^{-1}$ $\Delta H^\circ$
--	--

`thermodynamics` » `pre` =  $\{\langle text \rangle\}$  Default: `\changestate`  
 The symbol before the variable. Inserted in text mode.

`thermodynamics` » `superscript-left` =  $\{\langle text \rangle\}$  (initially empty)  
 The left superscript. Inserted in text mode.

`thermodynamics` » `superscript-right` =  $\{\langle text \rangle\}$  Default: `\standardstate`  
 The right superscript. Inserted in text mode.

`thermodynamics` » `superscript` =  $\{\langle text \rangle\}$   
 An alias of `superscript-right`.

`thermodynamics` » `subscript-left` =  $\{\langle text \rangle\}$  (initially empty)  
 The left subscript. Inserted in text mode.

`thermodynamics` » `subscript-right` =  $\{\langle text \rangle\}$  (initially empty)  
 The right subscript. Inserted in text mode.

`thermodynamics` » `subscript` =  $\{\langle text \rangle\}$   
 An alias of `subscript-left`.

**thermodynamics** » **subscript-pos** = left|right Default: left  
 Determines whether the subscript given in ( $\langle subscript \rangle$ ) is placed to the left or the right of the variable.

**thermodynamics** » **symbol** = { $\langle symbol \rangle$ } (initially empty)  
 The symbol of the variable. Inserted in math mode.

**thermodynamics** » **unit** = { $\langle unit \rangle$ } (initially empty)  
 A valid siunitx unit.

The default values depend on the command.

<pre>1 \enthalpy[unit=\kilo\joule]{-285} \par 2 \gibbs[pre=]{0} \par 3 \entropy[pre=\$\Delta\$,superscript   =]{56.7}</pre>	$\Delta H^\circ = -285 \text{ kJ}$ $G^\circ = 0 \text{ kJ mol}^{-1}$ $\Delta S = 56.7 \text{ J K}^{-1} \text{ mol}^{-1}$
---	--

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

<pre>1 \enthalpy{-1234.56e3} \par 2 \sisetup{ 3   per-mode=symbol, 4   exponent-product=\cdot, 5   output-decimal-marker={,}, 6   group-four-digits=true 7 } 8 \enthalpy{-1234.56e3}</pre>	$\Delta H^\circ = -1234.56 \times 10^3 \text{ kJ mol}^{-1}$ $\Delta H^\circ = -1\,234,56 \cdot 10^3 \text{ kJ/mol}$
--	--

### 7.10.3. Create New Variables or Redefine Existing Ones

**\NewChemState**{ $\langle cs \rangle$ }{ $\langle options \rangle$ }  
 Define new state commands like **\enthalpy**. Gives an error if  $\langle cs \rangle$  already exists.

**\RenewChemState**{ $\langle cs \rangle$ }{ $\langle options \rangle$ }  
 Redefine existing state commands.

**\DeclareChemState**{ $\langle cs \rangle$ }{ $\langle options \rangle$ }  
 Like **\NewChemState** but gives no error if  $\langle cs \rangle$  already exists.

**\ProvideChemState**{ $\langle cs \rangle$ }{ $\langle options \rangle$ }  
 Define new state commands like **\enthalpy**. Defines  $\langle cs \rangle$  only if it is not defined, yet.

The argument  $\langle options \rangle$  is a comma separated list of key/value options:

**thermodynamics** » **pre** = { $\langle text \rangle$ } Default: **\changestate**  
 The symbol before the variable.

**thermodynamics** » **superscript-left** = { $\langle text \rangle$ } (initially empty)  
 The left superscript.

- thermodynamics** » **superscript-right** =  $\{\langle text \rangle\}$  Default: `\standardstate`  
 The right superscript.
- thermodynamics** » **superscript** =  $\{\langle text \rangle\}$   
 An alias of **superscript-right**.
- thermodynamics** » **subscript-left** =  $\{\langle text \rangle\}$  (initially empty)  
 The left subscript.
- thermodynamics** » **subscript-right** =  $\{\langle text \rangle\}$  (initially empty)  
 The right subscript.
- thermodynamics** » **subscript** =  $\{\langle text \rangle\}$   
 An alias of **subscript-left**.
- thermodynamics** » **subscript-pos** = left|right Default: left  
 Determines whether the subscript given in ( $\langle subscript \rangle$ ) is placed to the left or the right of the variable.
- thermodynamics** » **symbol** =  $\{\langle symbol \rangle\}$  (initially empty)  
 The symbol of the variable.
- thermodynamics** » **unit** =  $\{\langle unit \rangle\}$  (initially empty)  
 A valid siunitx unit.

```

1 \NewChemState\Helmholtz{ symbol=A , unit=\kilo\joule\per\mole }
2 \NewChemState\ElPot{ symbol=E , subscript-pos=right , superscript= , unit=\volt
  }
3 \Helmholtz{123.4} \par
4 \ElPot{-1.1} \par
5 \ElPot[superscript=0]($\ch{Sn}||\ch{Sn^2+}||\ch{Pb^2+}||\ch{Pb}$){0.01} \par
6 \RenewChemState\enthalpy{ symbol=h , unit=\joule} \par
7 \enthalpy(f){12.5}

```

---


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

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

$$\Delta E^\ominus_{\text{Sn}|\text{Sn}^{2+}||\text{Pb}^{2+}|\text{Pb}} = 0.01 \text{ V}$$

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

The existing commands have been defined like this:

```

1 \NewChemState \enthalpy{ symbol = H, unit = \kilo\joule\per\mole }
2 \NewChemState \entropy { symbol = S, unit = \joule\per\kelvin\per\mole, pre = }
3 \NewChemState \gibbs { symbol = G, unit = \kilo\joule\per\mole }

```

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

```

1 \RenewChemState\enthalpy{symbol=h,superscript=,unit=\kilo\joule\per\mole}%
   molar
2 \RenewChemState\Enthalpy{symbol=H,superscript=,unit=\kilo\joule}% absolute
3 \enthalpy{-12.3} \Enthalpy{-12.3}

```

---

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

### 7.11. The units Module

The units module loads the siunitx package [Wri15].

In chemistry some non-SI units are very common. siunitx provides the command

`\DeclareSIUnit{<cs>}{<unit>}`

Define `<cs>` to be a valid unit command inside siunitx' macros `\SI` and `\si` which represents `<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`  
 $\text{cm}^3$

The units `\cmc`, `\molar`, and `\Molar` are defined by the package chemstyle as well. `CHEMMACROS` only defines them, if chemstyle is not loaded.

`\molar`  
 $\text{mol dm}^{-3}$

`\moLar`  
 $\text{mol L}^{-1}$

`\Molar`  
M

`\MolMass`  
 $\text{g mol}^{-1}$

`\normal`  
N

`\torr`  
torr

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

## 8. Internal Modules


### 8.1. The tikz Module

The tikz module loads the tikz package [Tan13] and the TikZ library calc.

#### 8.1.1. For Users

The tikz module defines a few arrow tips:

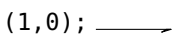
el

An arrow tip: `\tikz\draw[-el](0,0)--(1,0);` 

left el

An arrow tip: `\tikz\draw[-left el](0,0)--(1,0);` 

right el

An arrow tip: `\tikz\draw[-right el](0,0)--(1,0);` 

#### 8.1.2. For Module Writers

The tikz module provides some macros for common TikZ functions. This allows to use expl3's powerful function variants for expansion control.

`\chemmacros_other_colon_tl`

A constant tokenlist which contains a colon with category code 12 (other). This is useful since TikZ sometimes expects an other colon and in an expl3 programming environment : has category code 11 (letter).

`\chemmacros_tikz_picture:nn`  $\{\langle options \rangle\}$   $\{\langle code \rangle\}$

Defined as `\tikzpicture[{\#1}] #2 \endtikzpicture`.

`\chemmacros_tikz:nn`  $\{\langle options \rangle\}$   $\{\langle code \rangle\}$

Defined as `\tikz[{\#1}]{\#2}`.

`\chemmacros_tikz_draw:n`  $\{\langle options \rangle\}$

Defined as `\draw[{\#1}]`.

`\chemmacros_tikz_node:n`  $\{\langle options \rangle\}$

Defined as `\node[{\#1}]`.

`\chemmacros_tikz_shade:n`  $\{\langle options \rangle\}$

Defined as `\shade[{\#1}]`.

`\chemmacros_tikz_shadedraw:n`  $\{\langle options \rangle\}$

Defined as `\shadedraw[{\#1}]`.

`\chemmacros_tikz_node_in_draw:n`  $\{\langle options \rangle\}$

Defined as `node[{\#1}]`.

TABLE 4: Predefined xfrac text instances.

font family	text	superscript
cmr	$\frac{2}{3}$	$\frac{2}{3}$
lmr	$\frac{2}{3}$	$\frac{2}{3}$
LinuxLibertineT-TLF	$\frac{2}{3}$	$\frac{2}{3}$
LinuxLibertineT-T0sF	$\frac{2}{3}$	$\frac{2}{3}$

## 8.2. The xfrac Module

The xfrac module loads the package xfrac [L3Pb]. For the following explanations it will be helpful if you know about said package and how it works first. This module is a support module that defines the macro

`\chemfrac[⟨type⟩]{⟨numerator⟩}{⟨denominator⟩}`  
 ⟨type⟩ can either be text or superscript.

This macro calls a certain instance of the xfrac text template, depending on the option ⟨type⟩ and the current font family. If used `\chemfrac` looks if an instance

`chemmacros-frac-⟨family⟩-⟨type⟩`

exists. If yes this instance is used, if no the instance `chemmacros-frac-default-⟨type⟩` is used. The default instances are the same as the ones for cmr.

The xfrac module defines instances some font families, they are listed and demonstrated in table 4. The superscript type fractions *look* larger than the text types. The reason is that the superscript types are typically used with a smaller font size. Let's take a look at an example where both instances are used:

```

1 \chemsetup[redox]{pos=top}
2 \code{superscript}:
3 \ch{"\ox{1/3,I}" {}3+}
4
5 \chemsetup[redox]{pos=side}
6 \code{text}: \ox{1/3,I3+}
7
8 \huge
9 \chemsetup[redox]{pos=top}
10 \code{superscript}:
11 \ch{"\ox{1/3,I}" {}3+}
12
13 \chemsetup[redox]{pos=side}
14 \code{text}: \ox{1/3,I3+}
```

superscript:  $I_3^{+ \frac{1}{3}}$   
 text:  $I_3 + (\frac{1}{3})$

superscript:  $I_3^{+ \frac{1}{3}}$   
 text:  $I_3 + (\frac{1}{3})$

If you define instances for other families please feel free to submit them to me (see section) so they can be added to the xfrac module.



## Part IV.

# Appendix

### A. Own Modules

#### A.1. How To

If you have additional functionality which you think might be useful as a **CHEMMACROS** module then you can easily write one yourself. The module must be a file in a path where  $\text{\TeX}$  can find it following a certain naming scheme. The file for a module `foo` must be named `chemmacros.module.foo.code.tex`.

The first line in the file then should look similar to this:

```
1 \ChemModule{foo}{2015/07/14 description of foo}
```

This registers module `foo` which means **CHEMMACROS** will accept this file as a valid module.

Since **CHEMMACROS** is written using `expl3` `\ChemModule` starts an `expl3` programming environment. If you don't want that but rather want to write your module using traditional  $\text{\LaTeX}$  2 $\epsilon$  methods then use the starred variant:

```
1 \ChemModule*{foo}{2015/07/14 description of foo}
```

In both variants `@` has category code 11 (letter).

You should be aware that your module *will not be loaded* with `\usechemmodule{all}`! The pseudo-module `all` contains a manually maintained list of the modules that are loaded by it.

If you decide to write your module `foo` using `expl3` and add options you want to be able to set using `\chemsetup[foo]{<options>}` please make sure you define them the following way:

```
1 \keys_define:nn {chemmacros/foo} {  
2   ...  
3 }
```

Also (especially if you consider submitting the module, see section A.2) please follow the `expl3` naming conventions for variables and functions, *i. e.*, use `chemmacros` as `expl3` module name:

```
1 \tl_new:N \l__chemmacros_my_internal_variable_tl  
2 \tl_new:N \l__chemmacros_my_public_variable_tl  
3 \cs_new:Npn \__chemmacros_my_internal_function:n #1 { ... }  
4 \cs_new_protected:Npn \chemmacros_my_public_function:n #1 { ... }
```

```
5 \NewDocumentCommand \publicfunction {m}
6   { \chemmacros_my_public_function:n {#1} }
```

You will find more details on the naming conventions in `interface3.pdf` which most likely is available on your system:

```
~ $ texdoc interface3
```

## A.2. Submitting a Module

If you have written a module and feel it might be useful for other users please feel free to contact me and submit the module. I will surely take a look at both functionality and code and if I feel that it adds value to **CHEMMACROS** I will add it to the package. Requirement for this is that the module is licensed with the L<sup>A</sup>T<sub>E</sub>X Project Public License (v1.3 or later) and that I take over maintenance (according to the “maintainer” status of the L<sup>A</sup>T<sub>E</sub>X Project Public License).

Please do *not* submit your module via pull request but send me the files directly. In the best case you also have a short piece of documentation.

## B. Suggestions, Bug Reports, Support

**Support** If you need support or help with anything regarding **CHEMMACROS** please use the usual support forums

- <http://www.golatex.de/> or
- <http://texwelt.de/wissen/> if you speak German,
- <http://www.latex-community.org/forum/> or
- <http://tex.stackexchange.com/> if you speak English

or go the *dedicated support forum*

- <http://www.mychemistry.eu/forums/forum/chemmacros/>

where you can be sure that I will see the question.

**Suggestions** If you have any suggestions on how **CHEMMACROS** could be improved, adding missing features *etc.*, please feel free to contact me via [contact@mychemistry.eu](mailto:contact@mychemistry.eu).

**Bug reports** If you find any bugs, *i. e.*, errors (something not working as described, conflicts with other packages, ...) then please go to <https://github.com/cgnieder/chemmacros/issues/> and open a new issue describing the error including a minimal working example.

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