

# CHEMNUM

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numbering of chemical compounds

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## 1 License and Requirements

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 1.3c or later (<http://www.latex-project.org/lppl.txt>). The software has the status “maintained.”

CHEMNUM requires the bundles l3kernel [L3Pa] and l3packages [L3Pb]. It also requires the translations package [Nie20], chemgreek [Nie16] and the psfrag [GC98] package.

## 2 Overview over the Available Commands

This section lists all available commands with a brief description. Commands marked with *\** are expandable in an `\edef` like context. Most of the commands will be explained in a later section in more detail.

`\cmpd*+[\langle options \rangle]{\langle list of IDs \rangle}`

The main command for creating and referring to compound labels. This command is described in detail in section 4. For many people this will be the only command they need.

`\refcmpd[\langle options \rangle]{\langle ID \rangle}`

This command only refers to an already defined label but does not define a label itself. This is an alias of `\cmpd+`.

`\labelcmpd[\langle options \rangle]{\langle ID \rangle}`

This command only defines a new label but does not print it. This is an alias of `\cmpd*`.

*\** `\cmpdplain{\langle ID \rangle}`

Reads a label and writes it expandably without formatting. It is not able to parse a list. Its sole purpose is usage in PDF strings (cf. `\texorpdfstring{\langle TEX \rangle}{\langle PDF string \rangle}`). This command is described in section 4.

*\** `\subcmpdplain{\langle main ID \rangle}{\langle sub ID \rangle}`

Reads a sublabel and writes it expandably without formatting. It is not able to parse a list. Its sole purpose is usage in pdfstrings (cf. `\texorpdfstring{\langle TEX \rangle}{\langle PDF string \rangle}`). This command is described in section 4.

*\** `\submaincmpdplain{\langle main ID \rangle}{\langle sub ID \rangle}`

Reads a main label and a sublabel and writes them expandably without formatting. It is not able to parse a list. Its sole purpose is usage in PDF strings (cf. `\texorpdfstring{\langle TEX \rangle}{\langle PDF string \rangle}`). This command is described in section 4.

`\replacecmpd+[\langle options \rangle]{\langle ID \rangle}`

A command for replacing tags in EPS files, see section 8 for details.

`\initcmpd[\langle options \rangle]{\langle list of IDs \rangle}`

Initiate compound labels. This command can only be used in the preamble. It is described in section 4.

*\** `\cmpdproperty{\langle ID \rangle}{\langle property \rangle}`

Get the associated property `\langle property \rangle` of compound `\langle ID \rangle`. This command is described in section 4.

*\** `\subcmpdproperty{\langle main ID \rangle}{\langle sub ID \rangle}{\langle property \rangle}`

Get the associated property `\langle property \rangle` of subcompound `\langle sub ID \rangle` of compound `\langle main ID \rangle`. This command is described in section 4.

### 3 Numbering Compounds

`\newcmpdcounterformat{⟨name⟩}{⟨command⟩}`

Makes the label format  $\langle name \rangle$  known to `CHEMNUM`.  $\langle command \rangle$  needs to be a command that takes an integer number as argument and should return a formatted version of it. In practice you should not need to use this command as the most common formats already are defined. This command is described in section 6.1.

`\resetcmpd[⟨integer⟩]` Default: 1

Reset the numbering for main compound labels to start with  $\langle integer \rangle$  again. This is the same as `\setcounter{cmpdmain}{⟨integer⟩ - 1}`. The command is described in section 6.2.

`\cmpdshowdef{⟨ID⟩}`

Internal command used to display  $\langle ID \rangle$  of a newly defined compound label when the option `show-keys` is used. The command is described in section 11.

`\cmpdshowref{⟨ID⟩}`

Internal command used to display  $\langle ID \rangle$  of a referencing compound label when the option `show-keys` is used. The command is described in section 11.

`\subcmpdshowdef{⟨main ID⟩}{⟨sub ID⟩}`

Internal command used to display  $\langle main ID \rangle$  and  $\langle sub ID \rangle$  of a newly defined subcompound label when the option `show-keys` is used. The command is described in section 11.

`\subcmpdshowref{⟨main ID⟩}{⟨sub ID⟩}`

Internal command used to display  $\langle main ID \rangle$  and  $\langle sub ID \rangle$  of a referencing subcompound label when the option `show-keys` is used. The command is described in section 11.

`\setcmpdproperty{⟨property⟩}{⟨main ID⟩}{⟨value⟩}`

Sets property  $\langle property \rangle$  of compound  $\langle main ID \rangle$  to  $\langle value \rangle$ .

Introduced in  
version 1.3

`\setcmpdlabel{⟨main ID⟩}{⟨value⟩}`

Sets property counter-representation of compound  $\langle main ID \rangle$  to  $\langle value \rangle$ .

Introduced in  
version 1.3

## 3 Numbering Compounds

### 3.1 Main Command

The main command of this package is this one:

`\cmpd{⟨ID⟩}`

When  $\langle ID \rangle$  is used the first time, the label is created, saved (= declared) and printed. Each further use just prints the label.

- 1 Compounds `\cmpd{a}` and `\cmpd{b}` are declared and can be used any time:
  - 2 `\cmpd{a}`. No pre-declaring is necessary. Compounds like `\cmpd{c}` are
  - 3 numbered in the order they appear in the text. `\par`

### 3 Numbering Compounds

4 Once again: `\cmpd{b}`, `\cmpd{a}`, `\cmpd{c}`.

---

Compounds **1** and **2** are declared and can be used any time: **1**. No pre-declaring is necessary. Compounds like **3** are numbered in the order they appear in the text.

Once again: **2**, **1**, **3**.

If it is necessary to declare a compound without printing the label it is possible with

`\cmpd*{⟨ID⟩}`

Declare the label `⟨ID⟩` but don't print anything.

1 The hidden version `\cmpd*{d}` declares the label but doesn't print anything.  
2 The next `\cmpd{e}` continues to count with the next number. With `\cmpd{d}`  
3 the label can be used, of course.

---

The hidden version declares the label but doesn't print anything. The next **5** continues to count with the next number. With **4** the label can be used, of course.

You can pretty much use what you like for a label name except for the separator symbols (see also section 9). Be careful with blanks though! Leading and trailing spaces are ignored, spaces at other places are not. It's probably best not to use blanks in label names at all.

1 `\cmpd{aa}`, `\cmpd{aa_}`, `\cmpd{_aa}`, and `\cmpd{_aa_}` all have the same label.  
2 Likewise `\cmpd{a_a}`, `\cmpd{a_a_}`, `\cmpd{_a_a}`, `\cmpd{_a_a_}`, `\cmpd{a_aa}`,  
3 `\cmpd{a_aa_}`, `\cmpd{_a_aa}`, and `\cmpd{_a_aa_}`.

---

**6**, **6**, **6**, and **6** all have the same label. Likewise **7**, **7**, **7**, **7**, **7**, **7**, and **7**.

#### 3.2 Sublabels

If you want a label like **1a**, you need to use the following syntax:

`\cmpd{⟨main ID⟩.⟨sub ID⟩}`

`⟨main ID⟩` is the main name which stays the same, `⟨sub ID⟩` varies. This syntax means that the point `.` cannot be a part of `⟨main ID⟩` or `⟨sub ID⟩` (except if you enclose the respective ID in braces). Instead of the point you also can use another symbol, see section 9 for details.

### 3 Numbering Compounds

`\cmpd{f.one}` and `\cmpd{f.two}` are related, as are `\cmpd{g.one}` and `\cmpd{g.two}`. Of course these labels can be used again: `\cmpd{g.two}` and `\cmpd{f.one}`.

---

**8a** and **8b** are related, as are **9a** and **9b**. Of course these labels can be used again: **9b** and **8a**.

This also works if the main name has already been used.

`\cmpd{a}` and its variants `\cmpd{a.one}` and `\cmpd{a.two}`

---

**1** and its variants **1a** and **1b**

The same way the main name of combined labels can be used solely.

`\cmpd{f}` and `\cmpd{g}` **8** and **9**

How you can create a combined label like **8a,b** is explained in section 3.4.

#### 3.3 Lists

There is actually more to the `\cmpd` command. It also prints lists of labels. The right description would be something like:

`\cmpd{((possibly comma separated list of) label name(s))}`

Treats each entry of the list as described before.

This means that with default settings the comma can't be part of the label name unless hidden in braces. As separator another symbol can be used, too, see section 9 for details.

`\cs{cmpd}`, separated by commas. Then a list like `\cmpd{a, b, c, e, g.two}` is printed.

---

More than one label can be put inside `\compd`, separated by commas. Then a list like **1**, **2**, **3**, **5**, and **9b** is printed.

The Harvard comma (see section 10) in “, and” between **5** and **9b** suggests that there are options to customize the list, see section 7 for more on this.

The option `merge` has an effect on lists: if it is set to `true` multiple occurrences of a main label with a possibly different set of sublabels are merged into one label:

```
1 With \keyis{merge}{true} a list like \compd{c,g.two,a,g.{one,four}} looks
2 like \compd[merge=true]{c,g.two,a,g.{one,four}}.
```

---

With `merge = {true}` a list like **1**, **3**, **9b**, and **9a,c** looks like **1**, **3**, and **9b,a,c**.

### 3.4 Lists and Ranges of Sublabels

Sometimes it can be useful to display a label with a list or a range of sublabels. Suppose you have compounds **10a**, **10b**, **10c**, **10d**, and **10e** which for example differ in their substituents. It can be useful to refer to them all at once:

The syntax is rather intuitive – you just input a list of sublabels:

```
1 \setchemnum{compress=false}%
2 list of labels: \compd{q.one, q.two, q.three, q.four, q.five}\par
3 label with list of sublabels: \compd{q.{one,two,three,four,five}}
```

---

list of labels: **10a**, **10b**, **10c**, **10d**, and **10e**

label with list of sublabels: **10a,b,c,d,e**

Since the sublist is input with a comma in the default setting you have to put them into braces. If you add a list of sublabels to a main label they will always be printed in the order the sublabels have been declared and not in the order they're input in the list:

```
1 \setchemnum{compress=false}%
2 compare \compd{q.{one,two,three,four,five}}
3 with \compd{q.{five,four,three,two,one}} and
4 \compd{q.{three,four,one,five,two}}
```

### 3 Numbering Compounds

compare **10a,b,c,d,e** with **10e,d,c,b,a** and **10c,d,a,e,b**

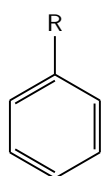
Using this syntax you also can create ranges of sublabels. For this you enable the option `compress`. Or rather: this is the default setting. If you don't want compressed sublabels you have to disable the option like in the previous examples.

```
1 \cmpd{q.{two,four,three}} \par 10b,d,c
2 \cmpd{q.{five,one,three,four}} \par 10e,a,c,d
3 \cmpd{q.{one,three,five,two}} 10a,c,e,b
```

Obviously you can't use a comma as part of a sublabel name. You can change the input marker, though. See section 5 for available options.

Sometimes it can be useful to get only the sublabel without the main label. This is achieved with the option `sub-only`:

```
1 % uses packages `chemfig', `chemformula' and `booktabs'
2 \chemname{\chemfig{*6(==(-R)-)}}{\cmpd{benzene.{H,Me,OH,NH2}}}
3 \quad
4 \begin{tabular}{lll}
5 \toprule
6 & & & & \ch{-R} & & Name \\
7 \midrule
8 \cmpd[sub-only]{benzene.H} & & \ch{-H} & & Benzene \\
9 \cmpd[sub-only]{benzene.Me} & & \ch{-CH3} & & Toluene \\
10 \cmpd[sub-only]{benzene.OH} & & \ch{-OH} & & Phenol \\
11 \cmpd[sub-only]{benzene.NH2} & & \ch{-NH2} & & Phenylamine (Aniline) \\
12 \bottomrule
13 \end{tabular}
```



**11a-d**

	-R	Name
<b>a</b>	-H	Benzene
<b>b</b>	-CH <sub>3</sub>	Toluene
<b>c</b>	-OH	Phenol
<b>d</b>	-NH <sub>2</sub>	Phenylamine (Aniline)

### 3.5 Usage in Section Headings and Captions

If you use labels in section headings or captions you will want to use either `\refcmpd` or `\cmpd+` (they are completely equivalent). Otherwise the corresponding labels will be declared when the section headings appear in the table of contents or maybe the page header. This would mess up the desired order of the compound numbers.

## 4 Details on Compound Labels

### 4.1 How Things Work

When you call `\cmpd` with a new label three things happen:

- The new label gets initiated. This is nothing more than adding it to an internal list. The purpose of this is explained in section 4.3.
- The new label gets declared. This means that a number of internal commands are defined. Amongst other things they hold a number of properties associated with the corresponding label. Those properties are explained in more detail in section 4.2. The necessary information of the label are also written to the aux file.
- The label gets printed.

Since new labels are declared when `\cmpd` is first used using it in section titles that are written to the table of contents may lead to wrong numbering. In order to avoid this compound label information is written to the aux file. The command `\refcmpd[options]{ID}` only reads those information but does not declare a label. There is also a command which does the opposite: it declares a label if it hasn't been declared before but will not print the corresponding label: `\labelcmpd[options]{ID}`. Both commands have shortcut versions: `\cmpd+` is the same as `\refcmpd`, `\cmpd*` is the same as `\labelcmpd`.

Another command available is `\cmpdplain{ID}`. This command is similar to `\refcmpd`. There are a few important differences, though: `\cmpdplain` does *not* take a list of labels as argument. It also is *not* able to interpret sublabels. `\cmpdplain` does not format the label with whatever format has been declared. And last but not least: it is expandable. This means it can be used to get labels in PDF bookmarks. Its equivalent `\subcmpdplain{main ID}{sub ID}` does the same for sublabels. A third sibling, `\submaincmpdplain{main ID}{sub ID}`, writes both the main and the sublabel.

I should also say a few words on lists of labels. A usage like `\cmpd{a, b, c, e}` will be printed as a *sorted* list. The order will be in the order *in which the labels have been defined*. The above usage gives **1, 2, 3, and 5**. The same thing holds for the order of sublabels of a compound: the usage `\cmpd{q. {one, three, four, two, five}}` gives **10a,c,d,b,e** or **10a,c,d,b,e** (depending on the `compress` option). Be careful if you have a list with several occurrences of the same main label but with different sublabels: the labels will not be sorted depending on their sublabels.



1	<code>\cmpd{q.five,q.two} \par</code>	<b>10e</b> and <b>10b</b>
2	<code>\cmpd{q.two,q.five} \par</code>	<b>10b</b> and <b>10e</b>
3	<code>\cmpd[merge]{q.five,q.two} \par</code>	<b>10e,b</b>
4	<code>\cmpd{q.five,b,r,q.two,a}</code>	<b>1, 2, 10e, 10b, and 12</b>

A last thing on lists: duplicate entries (*i. e.*, *exact* duplicates) will be removed.

## 4.2 Properties of Compound Labels

Every label has a number of properties. The first property is of course its ID which identifies the label. The other properties are:

**number** An internal unique number.

**counter-representation** The counter representation associated with the label. This is the actual label that get's printed.

**pre-label-code** Code to be inserted before the label is printed.

**post-label-code** Code to be inserted after the complete label is printed.

**pre-main-label-code** Code to be inserted before the *main* label is printed.

**post-main-label-code** Code to be inserted after the *main* label is printed.

**label-format** Formatting commands for the label. This is most likely something like `\bfseries`. This is the *default* format. Unlike the other properties it can be changed locally with the `format` option on a case by case basis.

The properties for a label are set the when a label is declared for the first time.

\* `\cmpdproperty{<ID>}{<property>}`

Get the associated property *<property>* of compound *<ID>*. This command is expandable.

```

1 \def\expandfull{\romannumeral-`0}%
2 \def\expandtwice{\detokenize\expandafter\expandafter\expandafter}%
3 \ttfamily
4 number: \cmpdproperty{benzene}{number}\par
5 counter-representation: \cmpdproperty{benzene}{counter-representation}\par
6 pre-label-code: \cmpdproperty{benzene}{pre-label-code}\par % empty
7 post-label-code: \cmpdproperty{benzene}{post-label-code}\par % empty
8 label-format: \expandtwice{\expandfull\cmpdproperty{benzene}{label-format}}
```

---

number: 11

#### 4 Details on Compound Labels

```
counter-representation: 11
pre-label-code:
post-label-code:
label-format: \protect \bfseries
```

Similarly a sublabel has associated properties. Additionally to the obvious ones – its ID and the ID the main label it belongs to – these are

**number** An internal unique number.

**counter-representation** The counter representation associated with the label. This is the actual label that gets printed.

\* `\subcmpdproperty{⟨main ID⟩}{⟨sub ID⟩}{⟨property⟩}`

Get the associated property *⟨property⟩* of subcompound *⟨sub ID⟩* of compound *⟨main ID⟩*. This command is expandable.

```
1 \ttfamily
2 main-compound: \subcmpdproperty{benzene}{OH}{main-compound}\par
3 number: \subcmpdproperty{benzene}{OH}{number}\par
4 counter-representation: \subcmpdproperty{benzene}{OH}{counter-representation}
```

---

```
main-compound: benzene
number: 3
counter-representation: c
```

If you compile with the `log = {verbose}` all properties of a label are listed in the log when it is declared. This will typically look like this:

```
1 .....
2 . chemnum info: defined new compound:
3 .   ID = a
4 .   internal number = 1
5 .   label = A
6 .   pre label code =
7 .   post label code =
8 .   pre main label code =
9 .   post main label code =
```

```

10 .   format = \bfseries
11 .....

```

### 4.3 Initiating Labels

Initiating labels is not the same as declaring them although it happens simultaneously. When a label is *initiated* its ID is added to an internal list. When a label is *declared* all of its properties and associated macros are defined. Initiating can serve two purposes:

1. It can help in keeping track of defined labels; if you set the option `init CHEMNUM` will either issue a warning or an error (depending on the actual setting you chose) if a label is used (and hence probably declared) *that hasn't been initiated*. This can also help in detecting typos in label names.
2. Since the labels are declared in the preamble you don't need to worry about a label erroneously being declared in the table of contents. This means the variants `\cmpd*` and `\cmpd+` shouldn't be needed.

Initiating is done via the command `\initcmpd`:

```

1 \initcmpd{a,b,c,d}

```

You simply use all IDs you want to use like you would use them in `\cmpd`. `\initcmpd` also has an optional argument that allows you to set options for those labels. Legal options are the same as for `\cmpd`.

Remember: `\initcmpd` will both initiate the labels *and* declare the labels!

## 5 Overview over the Available Options

All of the following options are either set as options to `\cmpd` or `\initcmpd` directly or via `\setchemnum{<options>}`, each time as a comma separated list of key/value pairs. Options that can only be set via `\setchemnum` are marked with `general`, those that only have an effect when used with `\cmpd` and friends are marked with `cmpd`. Those marked with `both` can be set either way. The options affecting the compounds are further divided in two classes: I named them global (`g`) and local (`l`). Options from the global class are set when a label is declared the first time and then are a fixed property of the corresponding label. Options from the local class can be changed at each instance of a label and will then only be active for the one instance.

A few of the options only have an effect when used with the `\replacecmpd` command. They are marked with `replace`.

`general` » `counter-within = {<counter>}`

Reset the compound numbers when `<counter>` is stepped.

## 5 Overview over the Available Options

- both (g)** » **counter-format** = arabic|alph|Alph|roman|Roman|greek|Greek Default: arabic  
 The format of the number associated with the main compounds.
- both (g)** » **sub-counter-format** = arabic|alph|Alph|roman|Roman|greek|Greek Default: alph  
 The format of the number associated with the sub compounds.
- both (l)** » **compress** = true|false Default: true  
 If set to true a list of sublabels is compressed, *i. e.*, **10a,c,d,e** becomes **10a,c-e**.
- both (l)** » **merge** = true|false Default: false  
 If set to true a list of labels is merged, *i. e.*, “**1, 10e, and 10b**” becomes “**1 and 10e,b**”.
- both (g)** » **pre-label-code** = {<code>} (initially empty)  
 Code to be inserted before a label.
- both (g)** » **post-label-code** = {<code>} (initially empty)  
 Code to be inserted after a label.
- both (g)** » **pre-main-label-code** = {<code>} (initially empty)  
 Code to be inserted before a main label.  
Introduced in version 1.2a
- both (g)** » **post-main-label-code** = {<code>} (initially empty)  
 Code to be inserted after a main label.  
Introduced in version 1.2a
- both (l)** » **main-sub-sep** = {<code>} Default: .  
 The separator symbol that is used in `\cmpd` to separate the <main ID> from a <sub ID>.
- both (l)** » **format** = {<formatting commands>} Default: \bfseries  
 The default format of the labels.
- both (l)** » **list-label-sep** = {<code>} Default: ,  
 The separator that is used to separate different <main IDs> in `\cmpd`.
- both (l)** » **sub-list-label-sep** = {<code>} Default: ,  
 The marker that is used to split an input list of sublabels.
- both (l)** » **list-sep-two** = {<code>} Default: \_and\_  
 The output separator between labels in a list that contains of two items.
- both (l)** » **list-sep-more** = {<code>} Default: ,\_  
 The output separator between labels in a list that contains of more than two items.
- both (l)** » **list-sep-last-two** = {<code>} Default: ,\_and\_  
 The output separator between the last two labels in a list that contains of more than two items.
- cmpd (l)** » **sub-only** = true|false Default: false  
 If true the command `\cmpd` will only print sublabels but no main labels.
- cmpd (l)** » **sub-all** = true|false Default: false  
 If true the command `\cmpd` will print all sublabels belonging to the corresponding main label.

## 5 Overview over the Available Options

- both (l)** » `sub-list-sep-two = {⟨code⟩}` Default: ,  
 The output separator between labels in a sublist that contains of two items.
- both (l)** » `sub-list-sep-more = {⟨code⟩}` Default: ,  
 The output separator between labels in a sublist that contains of more than two items.
- both (l)** » `sub-list-sep-last-two = {⟨code⟩}` Default: ,  
 The output separator between the last two labels in a sublist that contains of more than two items.
- both (l)** » `sub-list-sep-range = {⟨code⟩}` Default: --  
 The output separator between two labels in a sublist denoting a range. This is only used when the option `compress` is active.
- general** » `replace-auto = true|false` Default: true  
 When set to true this adds an incremented integer to the replacement tag.
- general** » `replace-tag = {⟨text⟩}` Default: TMP  
 The default replacement tag.
- general** » `replace-tag-nr = {⟨int⟩}` Default: 1  
 Introduced in version 1.1 The next number used by `\replacecmpd` when the default tag is used.
- replace** » `tag = {⟨text⟩}` Default: TMP⟨number⟩  
 The local replacement tag. `⟨number⟩` is incremented by one at each use and starts with 1. The starting number can be changed with the option `replace-tag-nr`. The increment happens locally.
- general** » `replace-style = {⟨code⟩}` Default: \sffamily  
 Additional  $\TeX$  code that it placed before the `\cmpd` command in the replacement.
- replace** » `style = {⟨code⟩}` Default: \sffamily  
 Local additional  $\TeX$  code that it placed before the `\cmpd` command in the replacement.
- general** » `replace-pos = {⟨ $\TeX$  pos⟩}{⟨PS pos⟩}` Default: bb  
 Options for `psfrag`'s `\psfrag`.
- replace** » `pos = {⟨ $\TeX$  pos⟩}{⟨PS pos⟩}` Default: bb  
 Local options for `psfrag`'s `\psfrag`.
- general** » `init = true|main|false|strict|main-strict` Default: false  
 Determines how labels have to be initiated. `false` means that labels are initiated when they're used the first time in the text. `true` means that labels should be initiated in the preamble with `\initcmpd`. `main` is the same as `true` but only for main labels. `strict` means that if an un-initiated label is used an error is thrown. `main-strict` is the same as `strict` but only for main labels.

**general** » `log = true|false|silent|verbose` Default: false

Determines how the declaration of the labels will be logged. `false` means that no information is written to the `.log` file. `true` means that basic information is written to the `.log` file when a label or a sublabel is declared. `silent` is an alias of `true`. `verbose` means that detailed information is written to the `.log` file when a label or a sublabel is declared.

**general** » `show-keys = true|false|def|ref` Default: false

This option will write visual hints when a label is defined (choices `true` or `def`) or when a label is referenced (choices `true` or `ref`).

**general** » `hyperlinks = true|false` Default: false

Introduced in  
version 1.2

When package `hyperref` is loaded and this option is set to `true` then each main label links back to the first time it has been used (*i. e.*, it has been labelled *and* printed).

## 6 The Counter Settings

The default setting for main labels is arabic numbering which is the most common use case for compound labels. There are however cases when you might want a different numbering. The numbering also is not reset in a document. I have heard of cases where this might be desirable, though. This section will tell you how you can achieve those things.

### 6.1 Change the Numbering

The counter representation used for the main and the sublabels can be changed using the following options:

**general** » `counter-format = arabic|alph|Alph|roman|Roman|greek|Greek` Default: arabic

The format of the number associated with the main compounds.

**general** » `sub-counter-format = arabic|alph|Alph|roman|Roman|greek|Greek` Default: alph

The format of the number associated with the sub compounds.

Those options can be set globally with `\setchemnum` or localized for the single compounds.

```
1 \compd[counter-format=Alph]{Alpha} and      M and ξ
2 \compd[counter-format=greek]{greek}
```

While it may not be necessary very often to change the default setting one could imagine cases where it makes sense, *e. g.*, Greek sublabels for the anomers of a carbohydrate.

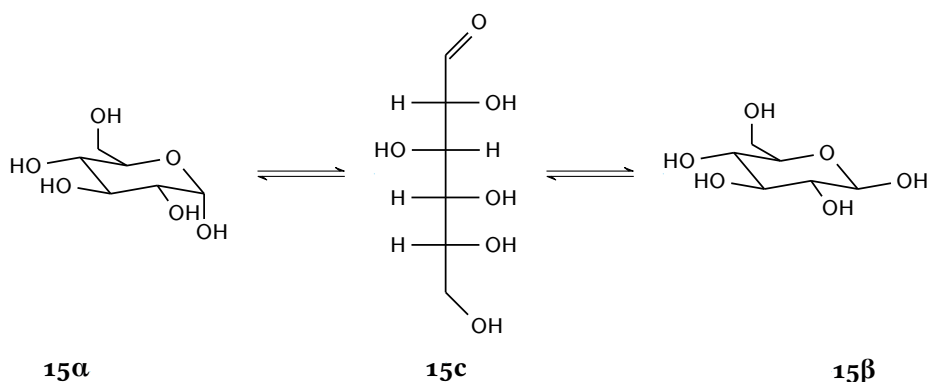
```
1 % this example uses the `chemfig' package
2 \definesubmol{r}{(-[4]H)(-[0]OH)}
```

## 6 The Counter Settings

```

3 \definesubmol{l}{(-[0]H)(-[4]HO)}
4 \labelcmpd[sub-counter-format=greek]{glucose.{alpha,beta}}
5 \labelcmpd{glucose.chain}
6 \centering
7 \schemestart
8   \small\chemfig{
9     ?(-[: -170]HO)
10    -[: -50](-[:170]HO)
11    -[:10](-[: -55,0.7]OH)
12    -[: -10](-[6,0.8]OH)
13    -[:130]O-[: -170]?(-[:150,0.7]-[2,0.7]OH)
14  }
15 \arrow(alpha--chain){<=>}
16 \small\chemfig{[6]O=^[5]-!r-!l-!r-!r--[7]OH}
17 \arrow(--beta){<=>}
18 \small\chemfig{
19   ?(-[: -170]HO)
20   -[: -50](-[:170]HO)
21   -[:10](-[: -55,0.7]OH)
22   -[: -10](-[:10]OH)(-[6,,,draw=none]\vphantom{OH})
23   -[:130]O-[: -170]?(-[:150,0.7]-[2,0.7]OH)
24 }
25 \arrow(@chain--chainlabel){0}[-90,.2] \cmpd{glucose.chain}
26 \arrow(@chainlabel--){0}[2.5] \cmpd{glucose.beta}
27 \arrow(@chainlabel--){0}[180,2.3] \cmpd{glucose.alpha}
28 \schemestop

```



Should it ever be necessary to use another kind of counter representations than the ones already provided they can be added with this command:

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

Makes the label format `<name>` known to `CHEMNUM`. `<code>` needs to end with a command that takes an integer number as mandatory argument and should return a formatted version of it.

The arabic and alph counter settings for example could have been defined like this:

```

1 \newcmpdcounterformat{arabic}{\@arabic}
2 \newcmpdcounterformat{alph} {\@alph}

```

This is actually not true: since `CHEMNUM` is written in `expl3` the corresponding `\int_to_<...>` functions have been used.

Although the name of the command suggests otherwise it can be used to overwrite the default definitions.

## 6.2 Reset the Numbering

There are cases when it actually might make sense to reset the counting of the compound labels. For this you can use this command:

```
\resetcmpd[<integer>] Default: 1
```

Reset the numbering for main compound labels to start with `<integer>` again. This is the same as `\setcounter{cmpdmain}{<integer> - 1}` which means the change is global!

Be careful, though. You might end up with the same number for different compounds:

```

1 \resetcmpd The numbering starts with 1 again: \cmpd{h,i,j}, but:
2 two compounds with the same label: \cmpd{a,h}

```

---

The numbering starts with 1 again: **1**, **2**, and **3**, but: two compounds with the same label: **1** and **1**

## 7 Formatting Labels

As you will have noticed by now labels are typeset with a bold face with the default setting of `CHEMNUM`. This can be changed:

```
both (1) » format = {<formatting commands>} Default: \bfseries
```

The default format of the labels.

This options works in two ways: it sets the default format that is picked up by a compound label when it is defined. When you change it later already defined labels dont change:

```

1 \setchemnum{format=\itshape} 1 and 2 and 4
2 \cmpd{a,b} and \cmpd{new}

```



## 7 Formatting Labels

If it is applied directly to the `\cmpd` command it changes the formatting for this usage of the command only, regardless if the label is new or not:

```
1 \cmpd[format=\itshape]{a,b} vs      1 and 2 vs 1 and 2
2 \cmpd{a,b}
```

There is more that you can do. Maybe you want to enclose labels in parentheses?

```
1 \cmpd[pre-label-code=(,post-label-code=)]{x, y, z.one }
```

---

(5), (6), and (7a)

Please note that these options only have an effect for *newly defined* labels since they belong to a label's properties.

Other options are the customization of the list separators:

**general** » `list-sep-two = {<code>}` Default: `_{and}_`

The output separator between labels in a list that contains of two items.

**general** » `list-sep-more = {<code>}` Default: `_{,}`

The output separator between labels in a list that contains of more than two items.

**general** » `list-sep-last-two = {<code>}` Default: `_{and}_`

The output separator between the last two labels in a list that contains of more than two items.

```
1 \setchemnum{list-sep-two=;,list-sep-more=;,list-sep-last-two=;}
2 \cmpd{a, b, c, d}
```

---

**1;2;3;4**

In the default settings these separators are language dependent. Setting them explicitly will overwrite the language sensitivity. If you only want to adapt the separators to your language have a look at section 10.

## 8 Replacing Tags in EPS or PS Files

Although it is quite possible to create reaction schemes within  $\text{\LaTeX}$  directly – for example with the `chemfig` package [Tel19] – many people prefer to use a program such as `CHEMDRAW` for it. In order to be able to use the labels with such schemes as well the following method is usually used:

- Create the scheme and place temporary tags like `TMP1`, `TMP2` and so on where you want the compound labels to be.
- Export the scheme as EPS or PS figure *where you make sure that the tags are embedded as text strings*. If the tags are not present as text strings they cannot be replaced. This is a common source of user problems.
- Include the EPS with `\includegraphics`. Right before that use `\replacecmpd` once for every temporary tag.

*For the actual replacement please make sure that you compile with `shell-escape` enabled. If you compile with `pdflatex` you probably also need `auto-pst-pdf` [RG09] loaded. In subsequent runs load it with option `off` when you turned off `shell-escape`.*

`\replacecmpd+[\langle options \rangle]{\langle ID \rangle}`

Replaces a tag in the following EPS file. This command doesn't have an optional star otherwise the syntax is the same as with `\cmpd`.

Figure 1 shows a scheme with temporary tags. It is produced with the following code where the class `standalone` has been used to get the figure only:

```

1 % code for figure 1
2 \documentclass{standalone}
3 \usepackage{graphicx,auto-pst-pdf}
4 \begin{document}
5   \includegraphics{scheme-tmp.ps}
6 \end{document}

```

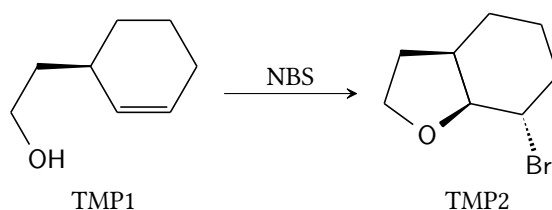


FIGURE 1: A scheme with temporary tags.

## 8 Replacing Tags in EPS or PS Files

The tags now can be replaced with labels. The result is shown in figure 2.

```
1 % code for figure 2 -- compiled with shell-escape enabled
2 \documentclass{standalone}
3 \usepackage{graphicx,auto-pst-pdf,chemnum}
4 \begin{document}
5   \replacecmd{Alc}% replaces TMP1
6   \replacecmd{EtherBr}% replaces TMP2
7   \includegraphics{scheme-tmp.ps}
8 \end{document}
```

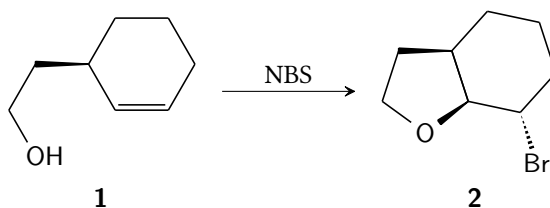


FIGURE 2: A scheme with temporary tags replaced with labels.

The replacement is done with the help of the `psfrag` package [GC98] and its `\psfrag` command. For details on this package and its command I refer to its documentation.

Although the examples don't do it the usage of `\replacecmd` and the corresponding graphic file should be placed inside a group (probably a `figure` or a `scheme` environment) in order to keep the stepping of the tag number local: this allows to use the same tags `TMP1`, `TMP2`, ..., in the next figure again.

As you can see the labels are printed sans serif. This setting can of course be changed. The complete list of options is this:

`general` » `replace-auto = true|false` Default: true

When set to true this adds an incremented integer to the replacement tag.

`general` » `replace-tag = {<text>}` Default: TMP

The default replacement tag.

`general` » `replace-tag-nr = {<int>}` Default: 1

Introduced in `version 1.1` The next number used by `\replacecmd` when the default tag is used.

`replace` » `tag = {<text>}` Default: TMP<number>

The local replacement tag. `<number>` is incremented by one at each use and starts with 1. The starting number can be changed with the option `replace-tag-nr`. The increment happens locally.

**general** » `replace-style = {⟨code⟩}` Default: `\sffamily`  
 Additional T<sub>E</sub>X code that it placed before the `\cmpd` command in the replacement.

**replace** » `style = {⟨code⟩}` Default: `\sffamily`  
 Local additional T<sub>E</sub>X code that it placed before the `\cmpd` command in the replacement.

**general** » `replace-pos = {⟨TEX pos⟩}{⟨PS pos⟩}` Default: `bb`  
 Options for psfrag's `\psfrag`.

**replace** » `pos = {⟨TEX pos⟩}{⟨PS pos⟩}` Default: `bb`  
 Local options for psfrag's `\psfrag`.

If you have a scheme with arbitrary tabs like in figure 3 you can specify the `tag` option to `\replacecmpd`. Figure 4 demonstrates this. It also demonstrates that you can of course use sublabels in the `\replacecmpd` command.

```

1 % code for figure 3
2 \documentclass{standalone}
3 \usepackage{graphicx,auto-pst-pdf}
4 \begin{document}
5   \includegraphics{scheme-bla.ps}
6 \end{document}

```

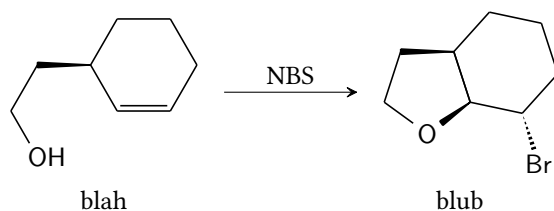


FIGURE 3: A scheme with arbitrary tags.

If you don't want to use `TMP⟨number⟩` as temporary tags but for example `temp⟨number⟩` you can change this with following option:

```

1 \setchemnum{replace-tag=temp}

```

The options `pos` and `replace-pos` refer to `\psfrag`'s optional arguments which determine the positioning of the T<sub>E</sub>X box with respect to the `ps` box that is replaced. This is described in psfrag's documentation.

## 9 Changing the Input Markers

```
1 % code for figure 4 -- compiled with shell-escape enabled
2 \documentclass{standalone}
3 \usepackage{graphicx,auto-pst-pdf,chemnum}
4 \begin{document}
5   \setchemnum{replace-style=\itshape}
6   \replacecmpd[tag=blah]{main}% replaces blah
7   \replacecmpd[tag=blub]{main.sub}% replaces blub
8   \includegraphics{scheme-bla.ps}
9 \end{document}
```

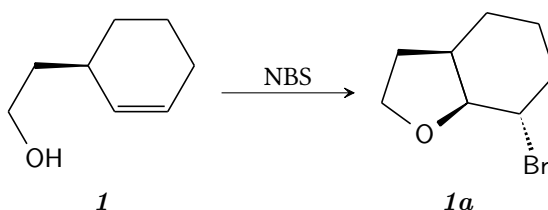


FIGURE 4: A scheme with arbitrary tags replaced with labels.

## 9 Changing the Input Markers

In **CHEMNUM**'s labels there are two markers (or three, actually) that can't be part of a label name: the comma , and the dot .. You can change them with options:

**general** » `list-label-sep = {<token>}` Default: ,  
The marker that is used to split an input list of main labels.

**general** » `sub-list-label-sep = {<token>}` Default: ,  
The marker that is used to split an input list of sublabels.

**general** » `main-sub-sep = {<token>}` Default: .  
The marker that divides sublabels from main labels.

```
1 \setchemnum{
2   main-sub-sep = ! ,
3   list-label-sep = ;
4 }
5 \cmpd{a; b; c; e; g!two} \par
6 \cmpd{q!one,two,three,four,five}
```

**1, 2, 3, 5, and 9b**  
**10a-e**

## 10 Language Dependent Settings

A few settings of `CHEMNUM` depend on the language you chose with `babel` [Bra19] or `polyglossia` [Cha19]. Those regard the list separators. The language dependent strings are translated with the help of the `translations` [Nie20] package. This package provides the means to define translations for strings associated with identification keys. `CHEMNUM` defines two strings. The available languages and the corresponding translations of the two strings are listed in table 1. Note that both the comma or a leading space as well as a trailing space are part of the translations. To make this obvious the relevant parts of the table are typeset in monospace and spaces are represented by `_`.

If you find your language missing or the translation to your language to be wrong please write me an email and I'll add your language or fix the wrong translation.

TABLE 1: Available languages

Language	<code>chemnum-sep-two</code>	<code>chemnum-sep-last-two</code>
English	<code>_and_</code>	<code>_and_</code>
American	<code>_and_</code>	<code>,_and_</code>
German	<code>_und_</code>	<code>_und_</code>
French	<code>_et_</code>	<code>_et_</code>
Spanish	<code>_y_</code>	<code>_y_</code>
Italian	<code>_e_</code>	<code>_e_</code>
Catalan	<code>_i_</code>	<code>_i_</code>
Portuguese	<code>_e_</code>	<code>_e_</code>
Dutch	<code>_en_</code>	<code>_en_</code>
Danish	<code>_og_</code>	<code>_og_</code>
Swedish	<code>_och_</code>	<code>_och_</code>
Finnish	<code>_ja_</code>	<code>_ja_</code>
Norwegian	<code>_og_</code>	<code>_og_</code>

## 11 Debugging Information

If you want information on the labels you have defined you can exploit the following options:

`general` » `log = true|false|silent|verbose` Default: `false`

Determines how the declaration of the labels will be logged. `false` means that no information is written to the `.log` file. `true` means that basic information is written to the `.log` file when a label or a sublabel is declared. `silent` is an alias of `true`. `verbose` means that detailed information is written to the `.log` file when a label or a sublabel is declared.

`general` » `show-keys = true|false|def|ref` Default: `false`

This option will write visual hints when a label is defined (choices `true` or `def`) or when a label is referenced (choices `true` or `ref`).

The option `log` will write information on a label to the `log` file when a label is defined. Depending on the choice (`true`, its alias `silent`, or `verbose`) this will be only the main information or detailed information including label properties. The following code shows an example when `log = {verbose}`:

```

1 .....
2 . chemnum info: defined new compound:
3 .   ID = a
4 .   internal number = 1
5 .   label = 1
6 .   pre label code = (
7 .   post label code = )
8 .   post main label code =
9 .   format = \bfseries
10 .....
```

The `show-keys` writes some visual information to the document itself:

```

1 \setchemnum{show-keys}
2 \cmpd{a} and a bit later \cmpd{b}.
```

---

<sup>a</sup>  
**1** and a bit later <sup>b</sup>  
**2**.

The last example shows the information when a label is referenced. If a label is newly declared information is written to the margin like for this label with the ID `showkey`: **8** that again is referenced here: **8**.

showkey

The option activates four commands:

`\cmpdshowdef{⟨ID⟩}`

Internal command used to display `⟨ID⟩` of a newly defined compound label when the option `show-keys` is used. The command is described in section 11.

`\cmpdshowref{⟨ID⟩}`

Internal command used to display `⟨ID⟩` of a referencing compound label when the option `show-keys` is used. The command is described in section 11.

`\subcmpdshowdef{⟨main ID⟩}{⟨sub ID⟩}`

Internal command used to display `⟨main ID⟩` and `⟨sub ID⟩` of a newly defined subcompound label when the option `show-keys` is used. The command is described in section 11.

`\subcmpdshowref{⟨main ID⟩}{⟨sub ID⟩}`

Internal command used to display  $\langle main ID \rangle$  and  $\langle sub ID \rangle$  of a referencing subcompound label when the option `show-keys` is used. The command is described in section 11.

This means you can customize the appearance of the information by redefining those commands. The ones that show the definition use a `\marginpar` in their default definition. This may cause them to disappear if issued somewhere `\marginpar` cannot be used. The following shows an equivalent definition with `\marginnote` from the `marginnote` package [Koh18]. (This definition has another drawback: it several `\marginnotes` can print over one another if issued in the same line.)

```

1 \renewcommand*\cmpdshowdef[1]{% /needs/ one mandatory argument
2   \marginnote{\fbox{\normalfont\ttfamily#1}}}
3 \renewcommand*\subcmpdshowdef[2]{% /needs/ two mandatory arguments
4   \marginnote{\fbox{\normalfont\ttfamily#2 (#1)}}}
5 a\cmpdshowdef{foo}\par
6 b\cmpdshowref{foo}\par
7 c\subcmpdshowdef{foo}{bar}\par
8 d\subcmpdshowref{foo}{bar}

```

---

```

a |foo
b |
c |bar
d |

```

foo

bar (foo)

Actually there are two other commands you could redefine – all four of the above commands are defined in terms of them:

```

1 \NewDocumentCommand\cmpdshowdef{m}{\chemnumshowdef{#1}}
2 \NewDocumentCommand\cmpdshowref{m}{\chemnumshowref{#1}}
3 \NewDocumentCommand\subcmpdshowdef{mm}{\chemnumshowdef{#2 (#1)}}
4 \NewDocumentCommand\subcmpdshowref{mm}{\chemnumshowref{#2}}

```

## 12 From Version 0 to Version 1

The `CHEMNUM` package has been my first attempt to create a comprehensive labeling package for chemical compounds. However, it had and has more than one weakness and its code was – to be frank – a mess. Version 1 is now a complete re-write of `CHEMNUM` where I tried to achieve several points:



## References

- A cleaner code internally.
- A cleaner user interface, *i. e.*, more user macros for different tasks, a unified naming of the commands and a less redundant naming of the options.
- Extended functionality such as sorting and compressing of sublabel lists and sorting and merging of main label lists.

Although the syntax seems more or less the same at first sight quite a number of changes have been made that make version 1 incompatible with version 0. While I thought a while about maintaining backwards compatibility version 0 was known to be in an experimental stage where everything was allowed to be changed at any time. So users *could* know there was a risk. I have a feeling that many users nevertheless didn't realize this and may be bothered by this incompatibility. So I am well aware that the update will inconvenience some users. However, since version 0 won't be updated any more it made more sense to make a breaking update once.

The same is not true for version 1. The syntax and commands described in this manual will not be changed as easily and from this version on I will take care of backwards compatibility.

For those people wanting to keep older versions: they are still available from websites such as [ctanhg.scharrer-online.de](http://ctanhg.scharrer-online.de) or [bitbucket.org/cgnieder/chemnum](http://bitbucket.org/cgnieder/chemnum). You can also email me for an older version.

Many commands have got a new name! The most important ones are:

- `\cmpdref`; this is now called `\replacecmpd`.
- `\cmpdinit`; this is now called `\initcmpd`.
- `\cmpdreset`; this is now called `\resetcmpd`.
- `\cmpdsetup`; this is now called `\setchemnum`.

However, there are many more changes. Basically all options have new names and often do their thing slightly different from the way things have been before.

Please note that this overall change does not mean that version 1 is version 0 declared stable. It is very likely that version 1 will now have quite a number of bugs to be fixed and probably missing features, too. So I'd be very glad to receive feedback either on **CHEMNUM**'s homepage [github.com/cgnieder/chemnum](https://github.com/cgnieder/chemnum) or via email to [contact@mychemistry.eu](mailto:contact@mychemistry.eu).

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