chemscheme — Support for chemical schemes *

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Released 2007/10/04

Abstract

The chemscheme package consists of two parts, both related to chemical schemes. The package adds a scheme float type to the LaTeX default types figure and table. The scheme float type acts in the same way as those defined by the LaTeX kernel, but is intended for chemical schemes. The package also provides a method for adding automatic chemical numbering to schemes.

Contents

1 Introduction

By default, LaTeX defines two float types, figure and table. Synthetic chemists make heavy use of schemes, which need a scheme float type. This is provided by chemscheme, in a manner consistent with the kernel floats.

*This file describes version v1.3, last revised 2007/10/04.

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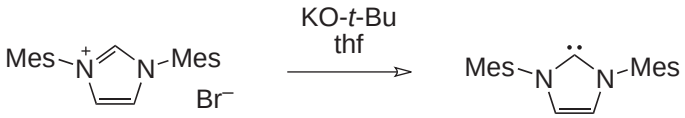
Synthetic chemists also number compounds for ease of reference. There are a number of LaTeX packages which cover this area, most notably `bpchem` and `chemcompounds`. However, adding numbers automatically to schemes is not covered by any existing package. The `chemscheme` package seeks to rectify this.

2 Floating schemes

2.1 Basic use

`scheme` The package provides a new float type, scheme, accessed in the usual way.

```
\begin{scheme}[ht]
  \includegraphics{scheme-one}
  \caption{A scheme with no compound numbers.}
\end{scheme}
```



Scheme 1: A scheme with no compound numbers.

The `scheme` float is designed to behave in the same way as the standard LaTeX float environments `figure` and `table`. Thus schemes will be placed at the top of a page, where possible. As shown in the example, the use of positional modifiers is allowed. Labelling and referencing schemes also follows the LaTeX conventions. `chemscheme` works hard to emulate the document class in use, and so the exact behaviour will depend on whether the standard classes, KOMA-SCRIPT or `memoir` are being used.

`\listofschemes` `\listschemename` To match the `\listoffigures` and `\listoftables` macros provided by the LaTeX kernel, `chemscheme` provides a `\listofschemes` command. This works in the same way as the kernel commands, with the default text stored in the macro `\listschemename`. Users upgrading from version 1.1 should note the change of macro name (from `\listscheme`). This is to bring `chemscheme` into line with the LaTeX kernel naming convention. Also notice that `\listofschemes` no longer accepts an optional argument. The standard output is illustrated below.

```
\listofschemes
```

List of Schemes

2.2 Altering the defaults

For users of the standard class files or the KOMA-SCRIPT bundle, the `float` package is used to create the new float type. Thus the usual `float` commands can be used to modify the behaviour as desired. Users of `memoir` will have slightly different commands available, as `memoir` implements its own new float mechanism, which is used in that case. Anything that you can do for a standard float, you should be able to to do for a scheme, and it should behave in the same way as a figure or a table. Please let the package maintainer know of any bugs in this support.

`\schemename` `\schemename` contains the text used in scheme captions (by default Scheme). This is used in the same manner as `\figurename` or `\tablename` to set up the text used in scheme captions.

```
\renewcommand*{\schemename}{Illustration}
\begin{scheme}[ht]
  \includegraphics{scheme-one}
  \caption{A scheme that is not a Scheme!}
\end{scheme}
```

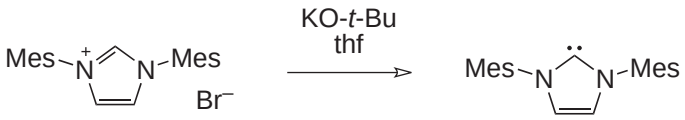


Illustration 2: A scheme that is not a Scheme!

2.3 `babel` support

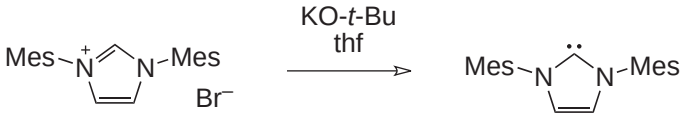
Schemes are provided with some support for `babel`. Currently, in addition to English, `chemscheme` provides alternatives for `\schemename` and `\listschemename` in French and German. Users of other languages are encouraged to supply suitable translations for inclusion in future versions of `chemscheme`.

3 Horizontal positioning of all floats

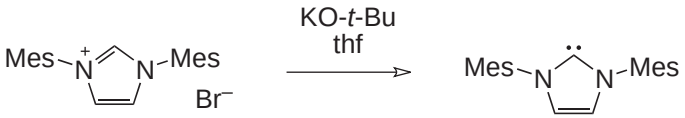
`\floatcontentscentre` `\floatcontentscenter` `\floatcontentsleft` `\floatcontentsright` The LaTeX default is to position all float contents flush-left. There is no "hook" provided to alter this. The `chemscheme` packages therefore provides commands to align all float contents automatically. As the macro names make clear, `\floatcontentscentre` will make all floats centred (for users speaking U.S. English, the alternative spelling `\floatcontentscenter` is also available). The

default behaviour is restored using the command `\floatcontentsleft`. Finally, `\floatcontentsright` is provided for use if needed. Notice that the float positioning commands should be given *outside* floating environments, and apply to all subsequent floats.

```
\floatcontentsleft
\begin{scheme}[ht]
  \includegraphics{scheme-one}
  \caption{A flush-left scheme.}
\end{scheme}
\floatcontentsright
\begin{scheme}[ht]
  \includegraphics{scheme-one}
  \caption{A flush-right scheme.}
\end{scheme}
\floatcontentscentre
```



Scheme 3: A flush-left scheme.



Scheme 4: A flush-right scheme.

It is important to note that the positioning mechanism used here relies on a low-level hack of the LaTeX kernel. This has been tested with the standard LaTeX classes, the memoir class and the KOMA-SCRIPT bundled. Other document classes may not give the desired behaviour.

4 Reference numbers in graphics

4.1 Background

There are a number of packages available on CTAN for tracking compound reference numbers. The two with the most up to date and comprehensive features are `bpchem` and `chemcompounds`. Both allow in-text numbering to be handled automatically. However, neither will allow the use of these numbers directly in schemes, figures, *etc.* Both leave it to the user to manually adapt schemes to match any changes in numbering.

The chemscheme package provides a mechanism for rectifying this issue. The package makes use of the psfrag package, which means that it can only directly produce DVI output (using LaTeX). However, direct PDF output using PDFLaTeX is possible: see Section 4.3.

\chemschemeref
\chemschemerefsub

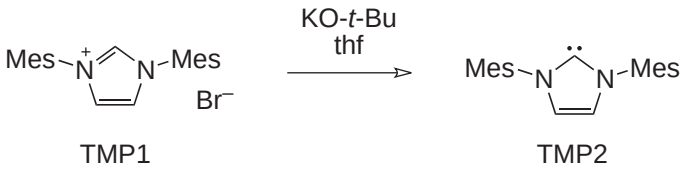
Users upgrading from v.2 should note that "chem" has been removed from the start of most macro names. The main referencing commands \chemschemeref and \chemschemerefsub are retained for backward compatibility.

4.2 Usage

Getting automated numbers into schemes is a two step procedure. In the first step, schemes (or other graphics) should be prepared as normal and saved as encapsulated postscript (EPS) files The most popular chemistry drawing package, ChemDraw, is able to do this from the Save As ... dialog. The positions where the auto-labels should be have to be marked in the EPS file. The marker should consist of an "indicator" that the text is to be replaced, followed by a reference number or letter. For automated substitution, the "indicator" text should be the same in all graphics; the value it is stored in \schemerefmarker, and has default value TMP. Thus the graphics should contain labels TMP1, TMP2, *etc*. A suitable unmodified graphic is shown in in the next example.

\schemerefmarker

```
\begin{scheme}[ht]
  \includegraphics{scheme-two}
  \caption{A scheme with temporary compound numbers.}
\end{scheme}
```



TMP1 TMP2

Scheme 5: A scheme with temporary compound numbers.

The value of \schemerefmarker may be altered as normal, so for example to use XXX as the indicator for replacement in all graphics, you would execute:

```
\renewcommand*{\chemeschemerefmarker}{XXX}
```

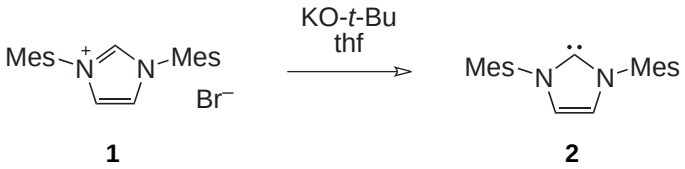
\schemeref

In the second step, the command \schemeref is used to indicate the mapping of the temporary markers to the automatically-managed numbering. The syntax of the command is \chemschemeref[⟨*temp-marker*⟩]{⟨*label*⟩}, where ⟨*temp-marker*⟩ is the marker used in the graphic, and ⟨*label*⟩ is the name assigned to the compound by the user. By default, chemscheme will assume that ⟨*temp-marker*⟩ consists of the marker plus a number, beginning at 1 and incrementing by 1 for each additional structure inside one float. Each replacement requires a separate \chemschemeref, all of which should appear before the relevant \includegraphics command.

An example will make usage clearer. In the example used in this document, the starting material is given label IMesHCl and the product is called IMes. As

is shown in the next example, in the EPS file these are labelled TMP1 and TMP2, respectively. The automated package defaults are used.

```
\begin{scheme}[ht]
  \schemeref{IMesHCl}
  \schemeref{IMes}
  \includegraphics{scheme-two}
  \caption{A scheme with automated compound numbers.}
\end{scheme}
```

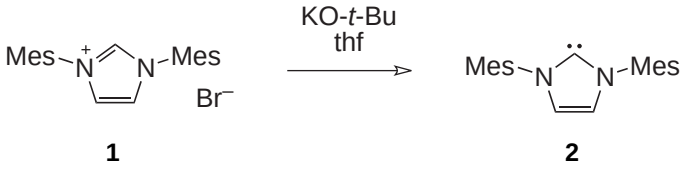


1 **2**

Scheme 6: A scheme with automated compound numbers.

With user-specified information on the text to be replaced, the entire text to be matched must be given.[1]

```
\begin{scheme}[ht]
  \schemeref[TMP1]{IMesHCl}
  \schemeref[TMP2]{IMes}
  \includegraphics{scheme-two}
  \caption{A scheme with explicitly numbered temporary labels.}
\end{scheme}
```



1 **2**

Scheme 7: A scheme with explicitly numbered temporary labels.

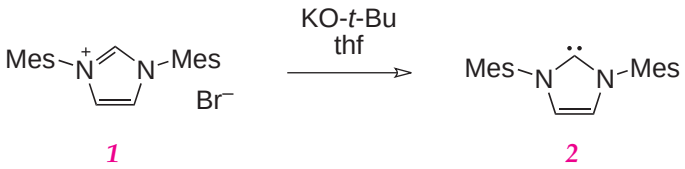
Notice that the new label is centred on the middle of the temporary marker, with the same baseline. This should allow the user to obtain good alignment of labels and structures.

`\schemerefsub` As described in Section 4.4, `chemscheme` supports `bpchem`, which allows tracking of sub-labels (**1a**, **1b**, *etc.*). To allow use of these in schemes, the `\schemerefsub` command is provided. This takes an additional argument {⟨*sub-label*⟩}, which is used to generate the appropriate text. When used with `chemcompounds`, this command will gobble its arguments and issue a warning; no substitution will take place.

`\schemerefformat` The format of chemical references is controlled by the underlying package, `bpchem` or `chemcompounds`. However, it is useful to be able to specify additional formatting for schemes. By default, `chemscheme` formats all reference numbers in a sans serif font. This is controlled by `\schemerefformat`.

[1] In this example, this is redundant as the automated system will work fine.

```
% This needs the color or xcolor package loaded
\renewcommand*{\schemerefformat}
  {\color{magenta}\textit}
\begin{scheme}[ht]
  \schemeref{IMesHCl}
  \schemeref{IMes}
  \includegraphics{scheme-two}
  \caption{A scheme with altered label formatting.}
\end{scheme}
```



1 *2*

Scheme 8: A scheme with altered label formatting.

The additional formatting applied within schemes may be altered by redefining `\schemerefformat`. By careful choice of the font commands given here, good visual matching should be obtained between the automatically-generated labels and other text in the scheme. In this document, the CHEMDRAW source uses 10 point Arial, with the LaTeX sans serif font provided by the `helvet` package, loaded scaled to 95 %, *i.e.*:

```
\usepackage[scaled=0.95]{helvet}
```

The CHEMDRAW file used to generate the example schemes is included with the package as `chemscheme.cdx`.

4.3 `chemscheme` and PDFLaTeX

The automatic substitution of numbers in graphics relies on the the `psfrag` package. This works with POSTSCRIPT files, and cannot therefore be used with PDFLaTeX. However, all is not lost as the `pst-pdf` package provides a method for including POSTSCRIPT files in a PDFLaTeX run. However, this is not automatic and some effort is needed by the user.[2] The example below shows a example for using PDFLaTeX with `chemscheme`.[3]

[2] The rest of this section is based closely on an example by Stefan Pinnow.

[3] This example is saved as `example.tex` when this documentation is compiled.

```
\documentclass{article}
\usepackage[T1]{fontenc}
\usepackage{graphicx,chemscheme}
% Remove inactive after the first LaTeX run
\usepackage[inactive,final]{pst-pdf}
\begin{document}
\floatcontentscentre
An example file for PDFLaTeX use.
\begin{scheme}
  \schemeref{IMesHCl}
  \schemeref{IMes}
  \includegraphics{scheme-two}
  \caption{A scheme with automated compound numbers.}
  \label{sc:scheme-one}
\end{scheme}
\end{document}
```

First you need to run the file through LaTeX, so your package can make the replacements in the picture. Then you need another run through LaTeX with the `inactive` option `pst-pdf` removed so that the modified pictures are extracted.[4] Do not worry that you end up with a very odd looking DVI! Then you have to convert the extracted pictures to PDF by the following commands

```
dvips -o \jobname-pics.ps \jobname.dvi
ps2pdf \jobname-pics.ps
```

This converts the modified graphics into PDF format. After this, you can use PDFLaTeX as normal for your schemes. Notice that you will have to repeat the process if you need to modify the schemes or numbering in any way.

4.4 Managing chemical numbering

The `chemscheme` package can use one of two packages for management of chemical numbering: `bpchem` and `chemcompounds`. As of v1.3, `chemcompounds` is the default package for managing reference numbers.[5] Both packages have advantages: `bpchem` allows the tracking of sub-references (very common in organic chemistry), whilst `chemcompounds` has a very well thought-out interface. It is technically feasible to support both simultaneously, but this is unlikely to have wide application. For this reason, `chemscheme` loads only one package (depending on the user option given), and uses this package to provide numbering management. Both `bpchem` and `chemcompounds` provide a variety of methods for defining chemical labels.

[4] You can simply do the first LaTeX run without loading `pst-pdf` at all, if you prefer.

[5] The change from `bpchem` is due to issues with `hyperref` support. The method used by `bpchem` to generate compound labels means that they are made into hyperlinks by `hyperref`, and therefore end up coloured when using the `colorlinks` option. This is unlikely to be the desired effect, and `chemcompounds` does not behave in this way.

5 Generating chemical schemes

5.1 Overview

There are a number of ways of generating the graphical content of schemes. The choice of method will depend on what is available to the user, and how complex the schemes desired are. In this section, an overview of several approaches is given.[6] The package author, who is a research worker in a university, favours using CHEMDRAW as it is regarded by many synthetic chemists as the best tool for this job. However, this is clearly overkill for users requiring a single diagram on a one-off basis. CHEMDRAW is also a commercial package running only under Windows and the MacOS. The following is necessarily somewhat brief and selective. For a thorough overview of graphics in LaTeX, see Goossens *et al.* [1].

5.2 Macro-based methods

At the most basic, a chemical scheme is simply a collection of lines and symbols, as with any vector diagram. Hence, it is possible to construct schemes directly using packages such as PSTricks or `pgf/tikz`. This is a complex method, and cannot be recommended for anyone except the very experienced and brave.

At a more practical level, there are two packages available which allow typesetting of chemical structures in (La)TeX, using specialised commands: XyMTeX and ppchTeX. Recent versions of the XyMTeX package have not been made available on CTAN, and the version held there is therefore considered to be obsolete. On the other hand, the ppchTeX system, developed originally for ConTeXt, is available. Both systems suffer from the lack of chemical logic in the input: it is very hard to tell from the code what is being represented. Drawing items such as "curly arrows", or making subtle alterations to positioning, is very challenging in purely macro-based systems. For these reasons, it is usually much more sensible to examine the available graphical methods.

5.3 Graphical methods

Moving to graphical systems, there is no reason that general-purpose vector drawing packages cannot be used for schemes. There are obviously several commercial (CORELDRAW, ADOBE ILLUSTRATOR, *etc.*) and freeware (for example the GIMP) drawing packages that can be used in this way. Simply rings and lines can easily be constructed, although in general-purpose programs the user has to watch that all bonds are the same length.

For producing a large number of complex schemes, the particular abilities of dedicated software become a necessity. As well as the already-mentioned CHEMDRAW, programs such as ISIS DRAW and CHEMSKETCH are available free for personal use;[7] these programs are all Windows specific. In the open-source arena, there are a number of packages such as XDRAWCHEM and BKCHEM, which offer cross-platform functionality. The differences between the various packages are in the ease of use, and ability to generate well-formattd output (for example, aligning structures).

[6] Thanks to Norwid-R. Behrnd for suggesting this section and giving a number of useful examples and tips.

[7] "Free" as in without charge, not as in open source.

One which deserves mention for the TeX user is TpX. This is a general purpose Windows graphics program specifically aimed at producing TeX-friendly output (such as PSTricks and `tikz` code) from a graphical interface. TpX can accept clipboard data from other programs, so can be used to produce EPS files from programs which do not have native export facilities (such as ISIS DRAW).

6 Known issues

The interaction of the different document classes, with options, plus the `babel` system means ensuring every possibility is covered is impossible. Users are asked to report any problems with compatibility with other packages or emulation of the standard float types. Additional `babel` stings are also welcome, as are improvements to those already provided.

7 Implementation

7.1 Setup code

The initial code goes through the usual steps of identifying the package.

```
\NeedsTeXFormat{LaTeX2e}
\ProvidesPackage{chemscheme}%
  [2007/10/04 v1.3 Support for chemical schemes]
```

The `psfrag` package is required to carry out the inclusion of chemical numbers in graphics. Robust patching of commands is provided by `elatex`. If the `memoir` package is not being used, the `float` package is used to provide support for new float types. However, if `memoir` is in use, `float` is not loaded. As `caption` makes things work very nicely too, we load that here if `memoir` is not in use.

```
\RequirePackage{psfrag,iflang}
\@ifclassloaded{memoir}{}
  {\RequirePackage{float,caption}}
```

Option processing now takes place. By default, `chemscheme` uses the `chemcompounds` package for managing chemical compound references. The options reflect this.

```
\newif  \ifchemsch@bpchem    \chemsch@bpchemfalse
\DeclareOption{chemcompounds}{\chemsch@bpchemfalse}
\DeclareOption{bpchem}{\chemsch@bpchemtrue}
```

The `chapter` option is no longer used, so the user is told that it is ignored. Hopefully nothing bad happens, and so an error is not appropriate.

```
\DeclareOption{chapter}%
  {\PackageInfo{chemscheme}%
  {Ignoring obsolete option 'chapter'}}
\ProcessOptions
```

7.2 Support for schemes

`\schemename` `\listschemename`

The default name for a scheme, and the default title for the list of schemes, are provided. Both command names follow the kernel conventions for figures and tables.

```
\newcommand*{\schemename}{Scheme}
\newcommand*{\listschemename}{List of Schemes}
```

scheme The `\newfloat` command is used to generate the new float type. The syntax depends on whether whether `float` or `memoir` is used for the definition. Notice that the formation of the new float has to wait for the beginning of the document, as this has to occur after `hyperref` may be loaded.

```
\@ifclassloaded{memoir}{%
```

In the `memoir` case, floats are always defined numbered within chapters.

```
  \AtBeginDocument{%
    \newfloat[chapter]{scheme}{los}{\schemename}
```

The `memoir` kernel makes various changes to the formatting of the default float types after they are declared. So the same is done here for schemes. The `\addtodef` macro is defined by `memoir`. Why all of this is done is not clear, but it is best to be on the safe side.

```
    \kill@lastcounter{losdepth}
    \renewcommand*{\thescheme}{\thechapter.\@arabic\c@scheme}
    \addtodef{\@smemfront}{}{\counterwithout{scheme}{chapter}}
    \addtodef{\@smemmain}{}{%
      \ifartopt\else
        \counterwithin{scheme}{chapter}
      \fi}
    \addtodef{\backmatter}{}{%
      \ifartopt\else
        \counterwithout{scheme}{chapter}%
        \setcounter{scheme}{0}%
      \fi}
    \ifartopt
      \counterwithout{scheme}{chapter}%
    \fi
  }
}{%
```

When using `float`, the standard LaTeX class behaviour is emulated. Only some classes define chapters, so this has to be tested and accounted for when forming the `scheme` float.

```
  \AtBeginDocument{%
    \@ifundefined{chapter}{%
      \newfloat{scheme}{tbp}{los}%
    }{%
      \newfloat{scheme}{tbp}{los}[chapter]
```

In the standard classes which do define chapters, a bit of hacking occurs with the labelling of floats. So the same is done for schemes. KOMA-SCRIPT doesn't do this, so a test is needed for that as well.

```
      \@ifundefined{KOMAScriptVersion}{%
        \renewcommand*{\thescheme}%
          {\ifnum\c@chapter>\z@ \thechapter.\fi \@arabic\c@scheme}
      }{}
```

To get the correct appearance for table of contents, the `\@chapter` macro is patched to recognise schemes. A bit of shuffling is required, since `\g@addto@macro` cannot be used here.

```
      \let\chemsch@orig@chapter\@chapter
      \def\chemsch@chapter{%
        \addtocontents{los}{\protect\addvspace{10\p@}}%
          \chemsch@orig@chapter}
      \let\@chapter\chemsch@chapter
    }
  }
}
```

\listofschemes

To ensure that things are labelled correctly, the new float type is given an appropriate name. Notice that `memoir` does this at the float-definition stage. In common with the standard float types, a `\listof` command is provided for schemes. Notice again the need for almost everything to take place after any potential loading of `hyperref`.

```
\@ifclassloaded{memoir}
  {\AtBeginDocument{%
    \newlistof{listofschemes}{los}{\listschemename}
```

Once again, various hacks are needed to get good emulation for `memoir`.

```
    \kill@lastcounter{losdepth}
    \newlistentry[chapter]{scheme}{los}{0}
    \cftsetindents{scheme}{0em}{2.3em}
    \addtodef{\insertchapterspace}{}%
      {\addtocontents{los}{\protect\addvspace{10pt}}}
    \@ifundefined{c@losdepth}%
      {\newcounter{losdepth}\setcounter{losdepth}{1}}{}%
    }
  }
```

For the standard document classes, things are a bit less complex. Notice that `\floatname` is needed to define the name of a scheme as "Scheme."

```
  {\floatname{scheme}{\schemename}
    \newcommand*{\listofschemes}{\listof{scheme}{\listschemename}}}
```

7.3 Positioning float contents

\floatcontentscentre
\floatcontentscenter
\floatcontentsleft
\floatcontentsright

In order to centre the content of all floats, a method is needed to break into the mechanism. None is provided by default, but it can be achieved by patching `\@floatboxreset`. User space switching commands are defined to turn centring on and off.

```
\newcommand*{\floatcontentscentre}%
  {\let\chemsch@everyfloat\centering}
\let\floatcontentscenter\floatcontentscentre
\newcommand*{\floatcontentsleft}%
  {\let\chemsch@everyfloat\relax}
\newcommand*{\floatcontentsright}%
  {\let\chemsch@everyfloat\raggedleft}
\let\chemsch@floatboxreset\@floatboxreset
\floatcontentsleft
\def\@floatboxreset{\chemsch@everyfloat\chemsch@floatboxreset}
```

7.4 `babel` support

To make the new float type work with `babel`, some alternative text is provided for non-English users. First, we need to know if `babel` is loaded *before* `chemscheme` or after, as this affects one if the hacks needed for French.

```
\newif  \ifchemsch@babel    \chemsch@babelfalse
\@ifpackageloaded{babel}
  {\chemsch@babeltrue}
  {}
```

There is then one hack to be made for French which has to be made before the beginning of the document *if* `babel` is loaded before `chemscheme`. This is only needed when `memoir` is not in use. So there is a run of tests to see if the conditions for the hack are met. `babel` support for French needs two name checks, *zut alors*!

```
\@ifclassloaded{memoir}
  {}
  {\@ifpackageloaded{babel}
  {\IfLanguageName{french}
    {\let\floatc@plain\FB@makecaption}
    {\IfLanguageName{frenchb}
      {\let\floatc@plain\FB@makecaption}
      {}}}
  {}}
```

The definition of new stings is delayed until the beginning of the document, so that things work if `babel` is loaded after `chemscheme`. The multiple language names mean quite a bit of repetition here.

```
\AtBeginDocument{%
  \@ifpackageloaded{babel}{%
    \addto{\captionsngerman}{\renewcommand*{\schemename}{Schema}}
    \addto{\captionsngerman}%
      {\renewcommand*{\listschemename}{Schemenverzeichnis}}
    \addto{\captionsgerman}{\renewcommand*{\schemename}{Schema}}
    \addto{\captionsgerman}%
      {\renewcommand*{\listschemename}{Schemenverzeichnis}}
```

French settings. `babel` also changes some style parameters here, so `chemscheme` tries to match this.

```
    \addto{\captionsfrench}%
      {\renewcommand*{\schemename}{\scshape Sch\'eme}}
    \addto{\captionsfrench}%
      {\renewcommand*{\listschemename}{Table des sch\'emes}}
    \addto{\captionsfrenchb}%
      {\renewcommand*{\schemename}{\scshape Sch\'eme}}
    \addto{\captionsfrenchb}%
      {\renewcommand*{\listschemename}{Table des sch\'emes}}
```

To make these changes, `babel` has to be instructed to reload the current language.

```
    \expandafter\selectlanguage\expandafter{\languagename}
```

If `babel` was loaded after `chemscheme`, and the document is in French, then the non-`memoir` patch for floats is needed here. This is the same one described earlier, which cannot be delayed to here if `babel` is loaded first.

```
    \@ifclassloaded{memoir}
      {}
```

```
      {\IfLanguageName{french}
        {\ifchemsch@babel\else
          \let\floatc@plain\FB@makecaption
        \fi}
        {\IfLanguageName{frenchb}
          {\ifchemsch@babel\else
            \let\floatc@plain\FB@makecaption
          \fi}
          {}}}
      {}
  }{}
}
```

7.5 Reference numbers in graphics

`\schemerefmarker` `\schemerefformat`

The two macros `\schemerefmarker` and `\schemerefformat` are used to allow customisation of the behaviour of the package. Here defaults are provided.

```
\newcommand*{\schemerefmarker}{TMP}
\newcommand*{\schemerefformat}{\textsf}
```

`\chemsch@label`

Depending on the user options provided, either `bpchem` or `chemcompounds` is loaded to manage chemical citations. The macro `\chemsch@label` is defined as the labelling command of the appropriate package.

```
\ifchemsch@bpchem
  \RequirePackage{bpchem}
  \let\chemsch@label\CNlabel
\else
  \RequirePackage{chemcompounds}
  \let\chemsch@label\compound
\fi
```

`\chemsch@num`

A counter is needed for automatic substitution of reference numbers. This has to be a TeX count, rather than a LaTeX counter, as it has to be local.

```
\newcount\chemsch@num
```

`\schemeref`

The user macro for referencing a compound in a graphic. First the automatic counter is incremented.

```
\newcommand*{\schemeref}{%
  \advance\chemsch@num\@ne%
```

Now the presence of an optional argument is tested for. If there is not one, the value of the automatic counter is used.

```
  \@ifnextchar[%
    {\chemsch@schemeref}
    {\chemsch@schemeref[\schemerefmarker\the\chemsch@num]}
}
```

`\chemsch@schemeref`

The internal command to substitute the temporary marker by the automatic label text. The use of `[b][b]` ensures that the new text is centred on the position of the marker.

```
\def\chemsch@schemeref[#1]#2{%
  \wlog{Replaing #1 by #2}%
```

```
  \psfrag{#1}[b][b]%
  {\schemerefformat{\chemsch@label{#2}}}%
}
```

\chemsch@schemerefsub For sub-referencing using bpchem, a similar macro is needed using the \CNlabelsub command. This is defined here, with the user macro later.

```
\def\chemsch@schemerefsub[#1]#2#3{%
  \psfrag{#1}[b][b]%
  {\schemerefformat{\CNlabelsub{#2}{#3}}}%
}
```

\chemschemeref The \chemschemeref is now a backward-compatibility wrapper for \schemeref.

```
\newcommand*{\chemschemeref}[1]{%
  \schemeref[#1]%
}
```

\schemerefsub \chemschemerefsub The user sub-referencing macro is defined in a package-dependent manner. If bpchem is loaded, then \schemerefsub works in the same way as \schemeref, but calling the sub version of the internal macro.

```
\ifchemsch@bpchem
  \newcommand*{\schemerefsub}{%
    \advance\chemsch@num\@ne%
    \@ifnextchar[%
      {\chemsch@schemerefsub}
      {\chemsch@schemerefsub[\schemerefmarker\the\chemsch@num]}
  }
```

Once again, backward compatibility is maintained.

```
  \newcommand*{\chemschemerefsub}[1]{%
    \schemerefsub[#1]%
  }
```

If chemcompounds is in use, then the sub-reference commands gobble the arguments given. The automatic counter is still incremented, so that things stay (reasonably) logical.

```
\else
  \newcommand*{\schemerefsub}[3][]{%
    \advance\chemsch@num\@ne%
    \PackageWarning{chemscheme}%
    {'chemcompound' option active\MessageBreak
      Command \protect\chemschemerefsub\space not used \MessageBreak
      Please alter your source to \MessageBreak
      \protect\chemschemeref}}
  \newcommand*{\chemschemerefsub}[1]{\schemerefsub}%
\fi
```

8 Change History

v1.0

v1.1

9 Index

Numbers written in italic refer to the page where the corresponding entry is described; numbers underlined refer to the code line of the definition; numbers in roman refer to the code lines where the entry is used.

10 References

[1] Michel Goossens, Frank Mittelbach, Sebastian Rahtz, and Denis Roegel. *The LaTeX Graphics Companion*. Tools and Techniques for Computer Typesetting. Addison Wesley, 2 edition, 2007.