

chemscheme — Support for chemical schemes ^{*}

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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.

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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.

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

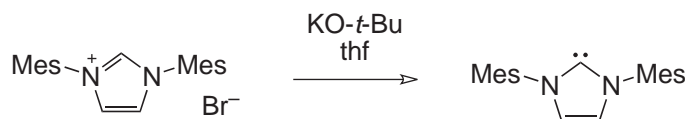
2.1 Basic use

`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}
```

The `scheme` float is designed to behave in the same way as the standard

Scheme 1: A scheme with no compound numbers.



\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.

List of Schemes

1	A scheme with no compound numbers.	3
2	A scheme that is not a Scheme!	4
3	A flush-left scheme.	5

4	A flush-right scheme.	5
5	A scheme with temporary compound numbers.	6
6	A scheme with automated compound numbers.	7
7	A scheme with explicitly numbered temporary labels.	7
8	A scheme with altered label formatting.	8

2.2 Altering the defaults

`floats` There are a number of methods available to generate new float types. The `memoir` class can do this internally, or the `float` or `floatrow` packages can be loaded to provide the necessary system. When `memoir` is used, `chemscheme` uses the internal systems for generating new floats; for the standard classes, `floatrow` is used by default. The `floats` package option can be used to control which method is employed. This uses the key-value system, can be given the values `float`, `floatrow` or `memoir`:

```
\usepackage[floats=float]{chemscheme}
```

or

```
\usepackage[floats=floatrow]{chemscheme}
```

or

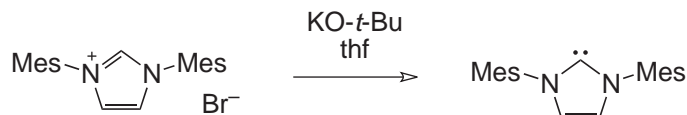
```
\usepackage[floats=memoir]{chemscheme}
```

The package will use the specified method if available (so `memoir` only works if using the `memoir` class!). If either `float` or `floatrow` is loaded before `chemscheme`, this forces the choice.

`\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.

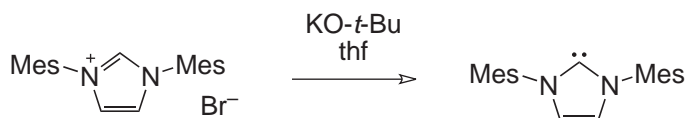
3 Horizontal positioning of all floats

`\floatcontentscentre`
`\floatcontentscenter`
`\floatcontentsleft`
`\floatcontentsright`

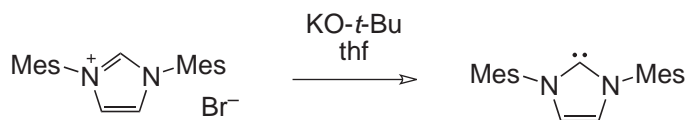
The \LaTeX default is to position all float contents flush-left. There is no “hook” provided to alter this. The chemscheme package therefore provides commands to align all float contents automatically. As the macro names make clear, `\floatcontentscentre` will make all floats centred (for users speaking 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.

`\chemscheme`
`\chemscheme`
`\chemscheme`

Users upgrading from v1.2 should note that “chem” has been removed from the start of most macro names. The main referencing commands `\chemscheme` and `\chemscheme` are retained for backward compatibility.

4.2 Usage

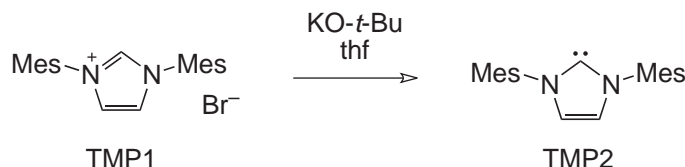
`\schemerefer`

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 `\schemerefer`, 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.

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

The value of `\schemerefer` may be altered as normal, so for example

Scheme 5: A scheme with temporary compound numbers.



to use `XXX` as the indicator for replacement in all graphics, you would execute:

```
\renewcommand*{\schemerefer}{XXX}
```

`\schemerefer`

In the second step, the command `\schemerefer` is used to indicate the map-

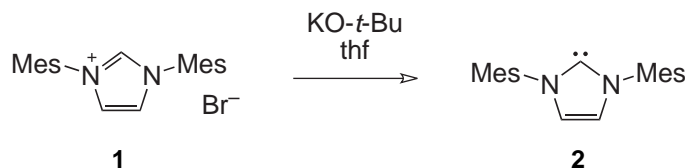
ping of the temporary markers to the automatically-managed numbering. The syntax of the command is `\chemschemeref[$\langle temp-marker \rangle$]{ $\langle label \rangle$ }`, where $\langle temp-marker \rangle$ is the marker used in the graphic, and $\langle label \rangle$ is the name assigned to the compound by the user. By default, chemscheme will assume that $\langle temp-marker \rangle$ 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}
```

With user-specified information on the text to be replaced, the entire text to

Scheme 6: A scheme with automated compound numbers.

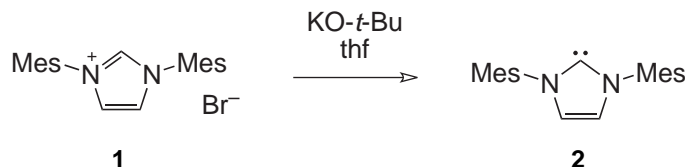


be matched must be given.¹

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

Notice that the new label is centred on the middle of the temporary marker, with

Scheme 7: A scheme with explicitly numbered temporary labels.



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

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

tracking of sub-labels (**1a**, **1b**, *etc.*). To allow use of these in schemes, the `\schemerefsb` command is provided. This takes an additional argument $\langle sub-label \rangle$, 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.

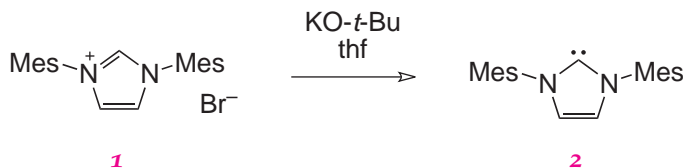
`\schemerefformat`

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`.

```
% 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}
```

The additional formatting applied within schemes may be altered by redefin-

Scheme 8: A scheme with altered label formatting.



ing `\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 PDF \LaTeX

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

```
1 \documentclass{article}
2 \usepackage[T1]{fontenc}
```

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


```

3 \usepackage{graphicx,chemscheme}
4 % Remove 'inactive' after the first LaTeX run
5 \usepackage[inactive,final]{pst-pdf}
6 \begin{document}
7 \floatcontentscentre
8 An example file for PDFLaTeX use.
9 \begin{scheme}
10   \schemeref{IMesHCl}
11   \schemeref{IMes}
12   \includegraphics{scheme-two}
13   \caption{A scheme with automated compound numbers.}
14   \label{sc:scheme-one}
15 \end{scheme}
16 \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.³ 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

bpchem
chemcompounds
tracking

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.⁴ 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, and uses this package to provide numbering management. The `chemscheme` package recognises the `bpchem` and `chemcompounds` to control this; the key-value version `tracking=...` can also be given.

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

³You can simply do the first \LaTeX run without loading `pst-pdf` at all, if you prefer.

⁴The 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.

the schemes desired are. In this section, an overview of several approaches is given.⁵ 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 L^AT_EX, 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 type-setting of chemical structures in (La)T_EX, using specialised commands: XyMT_EX and ppchT_EX. Recent versions of the XyMT_EX package have not been made available on CTAN, and the version held there is therefore considered to be obsolete. On the other hand, the ppchT_EX system, developed originally for ConT_EXt, 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;⁶ 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-formatted output (for example, aligning structures).

One which deserves mention for the T_EX user is TpX. This is a general purpose Windows graphics program specifically aimed at producing T_EX-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).

⁵Thanks to Norwid-R. Behrnd for suggesting this section and giving a number of useful examples and tips.

⁶“Free” as in without charge, not as in open source.

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` strings are also welcome, as are improvements to those already provided.

7 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.