chemstyle — Writing chemistry with style*

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Abstract

The chemstyle package provides a "one-stop shop" for setting up formatting of LaTeX documents following the editorial policies of various chemical journals. It provides a number of handy chemistry-related commands, and loads several support packages to aid the chemist.

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1 Introduction

The aim of chemstyle is to provide a quick method to set up various document parameters (such as caption formatting), simply by specifying the model journal. The package has also been designed to allow rapid addition of new journal styles. Each style definition is a separate file, and new styles can be added very readily. chemstyle has grown out of the rsc package, which had a similar aim but was much more limited (and less robustly implemented). The chemstyle package is also designed with the use of biblatex in mind: the rsc package is closely bound to traditional BibTeX use.

As a successor to the rsc package, chemstyle provides a range of chemistry-related additional macros. The set provided here is an extended version of those provide by rsc. Everything that can be done using the rsc LaTeX package is therefore possible using the chemstyle package.

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Table 1: Styles provided by chemstyle

Option	Journals using this style
none	Not applicable
angew	*Angew. Chem., Chem. Eur. J.*
jomc	*J. Organomet. Chem., Coord. Chem. Rev.*
ic	*Inorg. Chem.*
jacs	*J. Am. Chem. Soc.*
jcp	*J. Phys. Chem. A, J. Phys. Chem. B*
orglett	*Org. Lett.*
rsc	*Chem. Commun., Org. Biomol. Chem. Dalton Trans.*
tetlett	*Tetrahedron, Tetrahedron Lett.*

The formatting system provided by chemstyle are intended for writing a variety of documents. Thus the stylistic changes made by the package do not seek to reproduce the appearance of printed journal articles. The package aims to be suitable for use in preparing drafts of papers, but also for writing reports, theses and so on.

2 Style options for chemstyle

`journal` chemstyle should be loaded with a package option specifying which journal style to follow. Currently, chemstyle is aware of a the styles listed in Table 1. New styles can be developed by creating a new file modelled on the existing definitions; chemstyle will automatically search for correctly-named styles. The style files provided with chemstyle have been derived from current practice in the target journals. It is not always easy to pick the correct stylistic settings from (sometimes inconsistent) real-world examples. The package author welcomes feedback on the styles provided.

The `none` style is notable as it is not based on a journal. Instead this is a minimal style, which provides the additional commands without making formatting changes. It is also the default style if no option is given. This document has been compiled implicity using the `none` option, for example.

2.1 Creating styles

The process of creating a new styles for chemstyle is intended to be relatively easy. New styles should be saved as files with the extension `.jdf` (standing for for Journal Definition File), and should be saved somewhere in the path searched by TEX.[1] The definition files included in the package should provide a guide to the basic options available for producing new styles. Arbitrary TEX commands can be included, if they are necessary for a particular style. For example, other packages can be loaded in `\usepackage`.

[1] Depending on your TEX distribution, you may need to rebuild your file database after creating a new style. For MikTEX users, this can be done graphically or by typing `mpm -update-db` at the command line; for TeXLive, run `texhash`.

The maintainer of chemstyle is happy to add new styles to the package, either by contribution by users or on request (when he has sufficient time!). If you have a new style to add (or corrections to an existing one), please contact the package author.

2.2 Package options

journal

As of version 1.2, chemstyle uses the keyval system for option management. The choice of journal style can therefore be given as a normal option or by using the key `journal=`. The other package options provided by the package are described as they arise in the documentation.

\cstsetup

Some of the package options can only be set when loading the package. The choice of journal style is one of these. Others can be altered anywhere in the document, using the `\cstsetup` macro. This accepts a keyval list and processes it as needed.

chemcompounds
floatrow

chemstyle loads the chemscheme package, and therefore will pass through the `chemcompounds` option. It can also request floats are created either by float or floatrow; this is controlled by the `floatrow` option. Setting `floatrow=false` means that float is used to generate floats; the default value is **`true`**.

3 Naming of the references section

chemstyle alters the naming of the references section of a document. By default, chemstyle alters the value of `\bibname` or `\refname` (as appropriate) to the form of words chosen by the target journal for the "References" section.

The "Notes and References" naming commands are language-aware, *via* the babel interface. Currently, chemstyle includes appropriate labels for babel languages `english`, `UKenglish`, `ngerman` and `french`. Other languages can be added if appropriate wordings are provided to the author. The naming system is designed to work correctly with both natbib and biblatex.

notes
nonotes

The package recognises the `notes` option for controlling how the references section is named. The accepts the values `true`, `false` and `auto`. The Boolean values either enable or disable the addition of "Notes and" to the "References" of the section title. The `auto` option works in conjunction with the notes2bib package. If notes are added, "Notes and" is included in the section title, whereas if no notes are given the section title remains as "References". The `nonotes` option is equivalent to `notes=false`.

notesbefore

The second option for this area is `notesbefore`. This takes `true` and `false` only, and sets whether "Notes and References" or "References and Notes" is produced.

4 Additional macros

4.1 Additional units

\Hz
\mmHg
\molar
\Molar
\cmc

Both the SIunits and unitsdef packages provide methods for handling a range of units, but do not include a small number of unit macros useful to chemists. In contrast, the siunitx package provides all of these using the `synchem` module. If

Slunits or unitsdef are loaded, chemstyle provides the missing units. On the other hand, if no unit package is loaded, siunitx is loaded and provides the units itself.

10 Hz
20 mmHg
30 mol dm^{-3}
40 M
50 cm^3

```
\SI{10}{\Hz}\\
\SI{20}{\mmHg}\\
\SI{30}{\molar}\\
\SI{40}{\Molar}\\
\SI{50}{\cmc}
```

4.2 The standard state symbol

`\standardstate` Related to the above, but not exactly a unit is the `\standardstate` command.[2] This generates the tricky `\standardstate` symbol. The symbol will adapt to local sizing.

the standard conditions are indicated: $\ominus$
Common but not correct: $\Delta G_\mathrm{f}^\ominus$ or $\Delta G_\mathrm{f}{}^\ominus$
Better: $\Delta_\mathrm{f} G^\ominus$
Sizing: $\int_{T^\ominus}^{T_\mathrm{out}}$

```
the standard conditions are indicated: \standardstate\\
Common but not correct:
  $\Delta G_\mathrm{f}^\standardstate$ or
  $\Delta G_\mathrm{f}{}^\standardstate$ \\
Better:
  $\Delta_\mathrm{f}G^\standardstate$\\
Sizing:
  $\int^{T_{\mathrm{out}}}_{T^\standardstate}$
```

4.3 Alkyl radicals

`\nPr` `\iPr` `\nBu` `\iBu` `\sBu` `\tBu` There are a few alkyl radicals that come up all of the time. No one seems to have put these into a package, so they are provided here. As you would expect, `\iPr` gives *i*-Pr, `\iBu` gives *i*-Bu and `\tBu` gives *t*-Bu, and so on. The style of the output depends on the journal style specified; most journals seem to favour one version of the abbreviation.

The alkyl group could be *n*-Pr, *i*-Pr
or *n*-Bu without affecting the selectivity.

```
The alkyl group could be \nPr, \iPr\\
or \nBu without affecting the selectivity.
```

`xspace` When chemstyle is loaded using the `xspace` option, the xspace package is automatically used to add space after the command names, so that `\iPr group` will result in "*i*-Pr group" being typeset.

`radhyphen` `rademph` `radsuper` `radprefix` The appearance of these radical abbreviations is controlled by the package options `radhyphen`, `rademph`, `radsuper` and `radprefix`. The journal styles set these automatically, but they can be redefined at any point. The options work as might be expected, and are Boolean switches.

^{i}Pr ^{t}Bu
Bu-i Bu-s

```
\cstsetup{radhyphen=false,radsuper=true}\\
\iPr \tBu
\cstsetup{radhyphen=true,radsuper=false,%
  radprefix=false,rademph=false}\\
\iBu \sBu
```

4.4 Latin phrases

`\latin` `\etc` `\eg` `\ie` `\etal` The various Latin phrases commonly used in chemistry are made available as

the obvious commands. By altering the definition of `\latin`, this allows ready switching from italic to Roman typesetting. Notice that `\etc`, `\ie` and `\eg` are aware of trailing periods, and so doubling-up should not occur. Once again, these macros use xspace when given as a package option to handle automatic addition of spaces after these phrases.

`\invacuo`
`abbremph`

The use of italic for these abbreviations is set by altering the package option `abbremph`, which takes values `true` and `false`.

et al. or *in vacuo* plus *some text*
i.e. equals e.g. perhaps etc.

```
\etal or \invacuo plus \latin{some text}\\
\cstsetup{abbremph=false}
\ie equals \eg perhaps \etc
```

`abbrcomma`

For American journals, where it is obligatory to follow "*e.g.*" and "*i.e.*" with a comma, the package provides a mechanism for handling this automatically. Thus, when using an appropriate journal style, `\eg`, `\eg.` and `\eg,` will all result in typesetting "*e.g.*,". The Boolean package option `abbrcomma` controls this.

e.g. this
i.e., that

```
\eg this\\
\cstsetup{abbrcomma=true}
\ie that
```

The `\etc` and `\etal` commands are set up on the assumption that they come at the end of a sentence. Hence the spacing after these will default to an inter-sentence space. If you desire an inter-word space, use the normal methods

etc. more text
et al. have shown

```
\etc\ more text \\
\etal~have shown
```

`nophrases`

The definitions of all of the phrases are designed not to overwrite any given by the user *in the preamble*. So, if you have your own `\latin` macro, it will be used even if you load chemstyle. If you encounter any problems, try loading the package with the `nophrases` option; this option prevents the package even trying to define any of the phrase macros.

`\latinemphon`
`\latinemphoff`

For backward-compatibiltiy with previous versions of chemstyle, the macros `\latinemphon` and `\latinemphoff` are provided. These work as would be expected, to alter the formatting produced by `\latin`. The more general keyval method is now preferred for making this change.

5 Additional information

5.1 Advice for users of the rsc package

The chemstyle package is intended as a replacement for the rsc package. As such, it covers almost everything the the rsc LaTeX package does, and more. Users of rsc are strongly encouraged to update to using chemstyle. The bibliography styles provided by rsc will continue to be required, of course. Migration of these styles to biblatex is an on-going project.

[2] The `\standardstate` macro is only defined if the user does not have their own version.

5.2 Interactions with other packages

The chemstyle package has been designed to avoid, as far as possible, clashes with other packages. The package requires the presence of the standard graphicx and varioref packages. If these packages need to be loaded with explicit options, this should be done *before* loading chemstyle. The chemscheme package is also needed, as it provides the floating `scheme` environment essential in synthetic chemistry documents.

5.3 Captions above floats

The `scheme` float type is generated using either the float or floatrow package. This has the side-effect that the placement of captions for floats does not depended on where the `\caption` command comes inside the floating environment.[3] If you wish to alter the placement of captions, the mechanism of the underlying package will be needed. There are some subtle differences between the two: altough floatrow provides the float macros, they are not all 100% compatible. This document is compiled using floatrow, and so to fix the position of captions the following code is appropriate.

```
\begin{table}[ht]
  The float contents
  \caption{A caption below the float contents in the source}
\end{table}
\floatsetup[table]{style=plain} % When using floatrow
% \floatstyle{plain}
% \restylefloat{table} When using float
\begin{table}[ht]
  The second float contents, which should be above the caption
  \caption{A second caption below the float contents
    in the source}
\end{table}
```

Table 2: A caption below the float contents in the source

The float contents

The second float contents, which should be above the caption

Table 3: A second caption below the float contents in the source

6 A template for chemical articles

This is a very simple template for chemistry-related documents. Hopefully it contains a few extra hints for getting well-formatted documents quickly. For simplicity, the template assumes that the user is writing a thesis for a U.K. university. Hence it uses U.K. defaults and RSC-based styling. Most of the packages used

[3] Normally this is a good thing.

have good documentation, but a brief summary of why they are recommend follows.

```
\documentclass[fontsize=10pt,paper=a4,english,UKenglish]
  {scrreprt}
\usepackage{geometry,upgreek,booktabs,babel}
\usepackage[journal=rsc,xspace=true]{chemstyle}
\usepackage[version=3]{mhchem}
\usepackage[footnotes]{notes2bib}
\usepackage[final]{microtype}
\usepackage[final,inactive]{pst-pdf}
\usepackage[colorlinks]{hyperref}
\begin{document}
  Document contents go here
\end{document}
```

The versatile KOMA-script bundle provides more advanced versions of the standard document classes. If you want paragraphs separated out, with no indents (a common style for theses), add the `parskip` option to the font and paper size ones given here.

The babel system is loaded to sort out hyphenation and so on, and could be useful if there are any foreign-language quotes.

geometry allows the users to alter page layout with ease: much better than trying to hack the raw LaTeX system. booktabs gives much nicer looking tables than the LaTeX 2ε default. upgreek provides non-italic lowercase Greek letters, which should be used for things such as bond descriptions.

π-bond σ*-orbital `$\uppi$-bond $\upsigma^*$-orbital`

Load chemstyle (of course) to give not only some easy formatting, but also to automatically provide a float type for schemes, thanks to the chemscheme package. This also loads either chemcompounds or (optionally) bpchem to track compound numbers.

The mhchem package provides the `\ce` command for rapidly typesetting formulas, so that you can type `\ce{H2SO4}` and get H_2SO_4.[4]

The microtype package improves formatting when used with the pdfTeX engine. By giving the `final` option, it is active even when using `draft` as a global option.

Using notes2bib allows the user to automatically add notes to the bibliography from within the document body. So you can put `\bibnote{A note}` in the source, and this will move into the References section without any further effort. The `footnotes` option means that footnotes do the same.

Finally, the hyperref package makes headings, citations and so on into hyperlinks.

[4] There is a slight cheat here, as this document uses lower-case numerals in the text. The example is written as `$\ce{H2SO4}$`.