

chemstyle — Writing chemistry with style*

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Abstract

The chemstyle package provides a “one-stop shop” for setting up formatting of L^AT_EX 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 B^BT_EX 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 L^AT_EX package is therefore possible using the chemstyle package.

*This file describes version v1.3c, last revised 2008/08/18.

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Table 1: Styles provided by chemstyle

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

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 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 implicitly using the `none` option, for example.

2.1 Creating styles

The process of creating a new style for chemstyle is intended to be relatively easy. New styles should be saved as files with the extension `.jdf` (standing 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`.

¹Depending on your \TeX distribution, you may need to rebuild your file database after creating a new style. For Mik \TeX 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 <code>journal=</code> . 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 <code>\cstsetup</code> 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 <code>notes</code> option for controlling how the references section is named. The accepts the values <code>true</code> , <code>false</code> and <code>auto</code> . The Boolean values either enable or disable the addition of “Notes and” to the “References” of the section title. The <code>auto</code> option works in conjunction with the <code>notes2bib</code> 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 <code>nonotes</code> option is equivalent to <code>notes=false</code> .
notesbefore	The second option for this area is <code>notesbefore</code> . This takes <code>true</code> and <code>false</code> 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 Slunits 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 <code>synchem</code> 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	<code>\SI{10}{\Hz}\</code>
20 mmHg	<code>\SI{20}{\mmHg}\</code>
30 mol dm ⁻³	<code>\SI{30}{\molar}\</code>
40 M	<code>\SI{40}{\Molar}\</code>
50 cm ³	<code>\SI{50}{\cmc}\</code>

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:	the standard conditions are indicated: <code>\standardstate\</code>
\ominus	Common but not correct:
Common but not correct: ΔG_f^\ominus or ΔG_f^\ominus	<code>\$\Delta G_\mathrm{f}^\wedge\standardstate\$</code> or <code>\$\Delta G_\mathrm{f}^\wedge\standardstate\$ \</code>
Better: $\Delta_f G^\ominus$	Better:
Sizing: $\int_{T^\ominus}^{T^\text{out}}$	<code>\$\Delta_\mathrm{f}^\wedge G^\wedge\standardstate\$ \</code>
	Sizing:
	<code>\$\int_{T_\mathrm{out}}^{T_\mathrm{out}}\standardstate\$</code>

4.3 Alkyl radicals

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

These should also work inside the `\ce` macro of `mhchem` when if escaped mode:

n-Bu₂CH–C(*i*-Pr)₃ `\ce{\nBu$2CH-C(\iPr$)3}`

`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` 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.

<code>\iPr^tBu</code>	<code>\cstsetup{radhyphen=false,radsuper=true}\</code>
<code>Bu-iBu-s</code>	<code>\iPr \tBu</code>
	<code>\cstsetup{radhyphen=true,radsuper=false,%</code>
	<code>radprefix=false,rademph=false}\</code>
	<code>\iBu \sBu</code>

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

4.4 Latin phrases

`\latin` 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` 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 `\etal` or `\invacuo` plus `\latin{some text}\`
i.e. equals *e.g.* perhaps *etc.* `\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 `\eg` this`\`
i.e., that `\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 `\etc\` more text `\`
et al. have shown `\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` For backward-compatibility 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` L^AT_EX 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.

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 depend 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: although `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

³Normally this is a good thing.

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

```

1 \documentclass[fontsize=10pt,paper=a4,english,UKenglish]
2 {scrreprt}
3 \usepackage{geometry,upgreek,booktabs,babel}
4 \usepackage[journal=rsc,xspace=true]{chemstyle}
5 \usepackage[version=3]{mhchem}
6 \usepackage[footnotes]{notes2bib}
7 \usepackage[final]{microtype}
8 \usepackage[final,inactive]{pstr-pdf}
9 \usepackage[colorlinks]{hyperref}
10 \begin{document}
11 Document contents go here
12 \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 $\text{\LaTeX}_{\varepsilon}$ default. `upgreek` provides non-italic lowercase Greek letters, which should be used for things such as bond descriptions.

π -bond σ^* -orbital

$\text{\textcolor{blue}{\uppi}}\text{\textcolor{blue}{\$}}\text{-bond } \text{\textcolor{blue}{\upsigma}}^*\text{\textcolor{blue}{\$}}\text{-orbital}$

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 pdf\TeX 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.

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