

achemso — Support for submissions to American Chemical Society journals*

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Abstract

The `achemso` bundle provides a \LaTeX class file and \BibTeX style file in accordance with the requirements of the American Chemical Society (ACS). The files can be used for any documents, but have been carefully designed and tested to be suitable for submission to ACS journals.

The bundle also includes the `natmove` package. This package is loaded by `achemso`, and provides automatic moving of superscript citations after punctuation.

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1 Introduction

Support for \BibTeX bibliography following the requirements of the American Chemical Society (ACS), along with a package to make these easy to have been available since version one of `achemso`. The re-write from version 1 to version 2 made a number of improvements to the package, and also added a number of new features. However, neither version one nor version two of the package was targeted directly at use for submissions to ACS journals. This new release of `achemso` addresses this issue.

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The bundle consists of four parts. The first is a $\text{\LaTeX}_{2\epsilon}$ class, intended for use in submissions. It is based on the standard article class, but makes various changes to facilitate ease of use. The second part is the \LaTeX package. The package contains the parts of the bundle which are appropriate for use with other document classes.¹ Thirdly, two \BibTeX style files are included. These are used by both the class and the package, but can be used directly if desired. Finally, an example document is included; this is intended to act a potential template for submission, and illustrates the use of the class file.

2 Installation

The entire bundle is supplied with the TDS-ready ZIP file, `achemso.tds.zip`. Simply unzip this into your local texmf tree and run your hash program (`texhash` for \TeX Live or `initexmf -u` for \MiKTeX).

To extract the bundle of files from `achemso.dtx`, run $(\text{pdf})\text{\TeX}$ on `achemso.dtx`. This will produce all of the package files, and also `README.txt`. To extract the files and build the documentation, run $(\text{pdf})\text{\LaTeX}$ on `achemso.dtx`. The files can then be installed as above.

3 Requirements

The `achemso` class requires the following packages:

- `caption`
- `float`
- `natbib`
- `setspace`
- `xkeyval`

These are normally present in the current major \TeX distributions, but are also available from [The Comprehensive TeX Archive Network](#).

4 The class file

The class file has been designed for use in submitting journals to the ACS. It uses all of the modifications described here (those in the package as well as those in the class). The accompanying example manuscript can be used as a template for the correct use of the class file. It is intended to act as a model for submission.

When submitting communications to *J. Am. Chem. Soc.*, the class will automatically lay the document out in the publication style. This allows the author to judge the length of text submitted more accurately. Changing the manuscript in the demonstration document to communication will illustrate the effect.

¹For example, when writing a thesis.

4.1 Class options

- `journal` The class supports a limited number of options, which are specifically-targeted at submission. The class uses the `keyval` system for options, in the form `key=value`. The most important option is `journal`. This is the name of the target journal for the publication. The package is designed such that the choice of journal will set up the correct bibliography style and so on. The journals currently recognised by the package are summarised in [1](#). If an unknown journal is specified, the package will fall-back on the `journal=jacsat` option.
- `manuscript` The second option is the `manuscript` option. This specifies the type of paper in the manuscript. The values here are `article`, `note`, `communication`, `review`, `letter` and `perspective`. The valid values will depend on the value of `journal`. The `manuscript` option determines whether sections and an abstract are valid. The value `suppinfo` is also available for supporting information.
- Other options are provided by the package, but when used with the class these are silently ignored.

4.2 Manuscript meta-data

- `\author` Inspired by REVTeX, the `achemso` class alters the method for adding author information to the manuscript. Each author should be given as a separate `\author` command. These should be followed by an `\affiliation`, which applies to the preceding authors. The `\affiliation` macro takes an optional argument, for a short version of the affiliation.² At least one author should be followed by an `\email` macro, containing contact details. All authors with an e-mail address are automatically marked with a star. The example manuscript demonstrates the use of all of these macros. Notice that `\alsoaffiliation` is used when one (or more) authors work at multiple institutions, while `\altaffiliation` is intended for previous addresses (or other notes). Only `\affiliation` applies to multiple authors: both `\alsoaffiliation` and `\altaffiliation` are set on a per author basis.

```
\author{Author Person}
\author{Second Bloke}
\email{second.bloke@some.place}
\affiliation[University of Sometown]
    {University of Somewhere, Sometown, USA}
\altaffiliation
    {Previous address: Minute University, Nowhereville, USA}
\author{Indus Trialguy}
\email{i.trialguy@sponsor.co}
\affiliation[SponsoCo]
    {Research Department, SponsorCo, BigCity, USA}
\alsoaffiliation{University of Somewhere, Sometown, USA}
```

- `\and` The method used for setting the meta-data means that the normal `\and` and `\thanks` macros are not appropriate in the `pkgachemso` class. Both produce a warning if used.

The meta-data items should be given in the preamble to the L^AT_EX file, and no `\maketitle` macro is required in the document body. This is all handled by

²This will usually be the university or company name.

<i>Journal</i>	<i>Setting</i>
<i>Acc. Chem. Res.</i>	achre4
<i>ACS Chem. Biol.</i>	acbcct
<i>ACS Nano</i>	ancac3
<i>Anal. Chem.</i>	ancham
<i>Biochemistry</i>	bichaw
<i>Bioconjugate Chem.</i>	bcches
<i>Biomacromolecules</i>	bomaf6
<i>Biotechnol. Prog.</i>	bipret
<i>Chem. Res. Toxicol.</i>	crtoec
<i>Chem. Rev.</i>	chreay
<i>Chem. Mater.</i>	cmatex
<i>Cryst. Growth Des.</i>	cgdefu
<i>Energy Fuels</i>	enfuem
<i>Environ. Sci. Technol.</i>	esthag
<i>Ind. Eng. Chem. Res.</i>	iecred
<i>Inorg. Chem.</i>	inoraj
<i>J. Agric. Food Chem.</i>	jafcau
<i>J. Chem. Eng. Data</i>	jceaax
<i>J. Chem. Inf. Model.</i>	jcisd8
<i>J. Chem. Theory Comput.</i>	jctcce
<i>J. Comb. Chem.</i>	jcchff
<i>J. Med. Chem.</i>	jmcmar
<i>J. Nat. Prod.</i>	jnprdf
<i>J. Org. Chem.</i>	joceah
<i>J. Phys. Chem. A</i>	jpcafh
<i>J. Phys. Chem. B</i>	jpcbfk
<i>J. Phys. Chem. C</i>	jpccck
<i>J. Proteome Res.</i>	jprobs
<i>J. Am. Chem. Soc.</i>	jacsat
<i>Langmuir</i>	langd5
<i>Macromolecules</i>	mamobx
<i>Mol. Pharm.</i>	mpohbp
<i>Nano Lett.</i>	nalefd
<i>Org. Lett.</i>	orlef7
<i>Org. Proc. Res. Dev.</i>	oprdfk
<i>Organometallics</i>	orgnd7

Table 1: Values for journal option

the class file directly. At least one author, affiliation and e-mail address must be specified.

4.3 Floats

`scheme` The class defines three new floating environments: `scheme`, `chart` and `graph`.
`chart` These can be used as expected to include graphical content. The placement of
`graph` these new floats and the standard `table` and `figure` floats is altered to be “here” if possible. The contents of all floats is automatically horizontally centred on the page.

Cross-referencing to floats automatically includes the name of the floating environment. For example, `\ref{table:one}` will yield “Table 1” without the user adding the “Table” part.

4.4 Section headers

`\SectionNumbersOff` Some journals have no section numbering by default. This can be set up in
`\SectionNumbersOn` the appropriate configuration file, but it may be that individual users need to change the decision. The macros `\SectionNumbersOff` and `\SectionNumbersOn` are therefore available: these should be given in the preamble.

`\SectionsOff` More radically, the entire availability of sections can be turned on and of. This
`\SectionsOn` is functionality is available to the user *via* the `\SectionsOn` and `\SectionsOff` macros, which again are preamble-only.

`\AbstractOff` Similar functions are available for the abstract: `\AbstractOff` and `\AbstractOn`.
`\AbstractOn`

4.5 Special sections

`acknowledgement` The sections for acknowledgements and supporting information have dedicated
`suppinfo` environments available. These ensure that the section headings are generated, and that the text is sized corrected when using creating a Communication.

```
\begin{acknowledgment}
  The authors thank A.N.-Other.
\end{acknowledgment}

\begin{suppinfo}
  Full characterization data for all new compounds.
  This material is available for download from
  \url{http://pubs.acs.org}
\end{suppinfo}
```

`tocentry` For generating an entry for the graphical table of content, required by some journals, the environment `tocentry` is available. This prints its content in an appropriately sized box on a separate page. In contrast to the rest of the manuscript, this section is intended to be “print ready” in appearance.

```
\begin{tocentry}
  \includegraphics{toc-entry-graphic}
  Some text to explain the graphic.
\end{tocentry}
```

5 The package file

The `achemso` package is independent of the `class` file, and contains parts of the bundle useful outside of submission to the ACS.

5.1 Package options

As with the class options, the package uses the key–value method for option set up. These are used to control the output of citations and bibliographic data. The same options are used when creating journal configurations for the class: this is a task most users will not need to undertake!

<code>super</code>	The <code>super</code> option affects the handling of superscript reference markers. The option switches this behaviour on and off (and takes Boolean values: <code>super=true</code> and <code>super=false</code> are valid).
<code>maxauthors</code> <code>usetitle</code>	The <code>maxauthors</code> and <code>usetitle</code> options change the output of the <code>BibTeX</code> style files. <code>maxauthors</code> is the number of authors allowed before truncation to “et al.” occurs. The default is 15, but can be increased (for example for supplementary information). Using the value 0 means that all authors will be added to the list. The <code>usetitle</code> option is a Boolean, and sets whether the title of a paper referenced appears in the bibliography. The default is <code>usetitle=false</code> .
<code>biblabel</code>	Redefining the formatting of the numbers used in the bibliography usually requires modifying internal <code>LaTeX</code> macros. The <code>biblabel</code> option makes these changes more accessible: valid values are <code>plain</code> (use the number only), <code>brackets</code> (surround the number in brackets) and <code>period</code> or <code>fullstop</code> (follow the number by a full stop/period).
<code>biochem</code> <code>biochemistry</code>	Most ACS journals use the same bibliography style, with the only variation being the inclusion of article titles. However, a small number of journals use a rather different style; the journal <i>Biochemistry</i> is probably the most prominent. The <code>biochemistry</code> or <code>biochem</code> option uses the style of <i>Biochemistry</i> for the bibliography, rather than the normal ACS style. For this style, the <code>usetitle=true</code> option is the default. ³

5.2 Bibliography notes

<code>\bibnote</code> <code>\bibnotemark</code> <code>\bibnotetext</code>	<code>achemso</code> provides the <code>\bibnote</code> macro. This is intended for addition of notes to the bibliography (references). The macro accepts a single argument, which is transferred to the bibliography by <code>BibTeX</code> . In analogy to <code>\footnote</code> , the macros <code>\bibnotemark</code> and <code>\bibnotetext</code> are available for dividing up the marker for a note from the text.
---	---

Some text `\bibnote{This note text will be in the bibliography}`.
Some text.¹

The functionality for bibnotes in `achemso` is based on that in the `notes2bib` package. The `notes2bib` package can be loaded with the `achemso` package, and no clash will occur. With the class file, `notes2bib` will be ignored if requested, to prevent issues on submission to the ACS.

³More accurately, the default built into the `BibTeX` style file is to use article titles with the *Biochemistry* style.

6 The BibT_EX style files

achemso is supplied with two style files, `achemso.bst` and `biochem.bst`. The direct use of these without the `achemso` package file is not recommended, but is possible. The style files can be loaded in the usual way, with a `\bibliographystyle` command. The `natbib` package must be loaded by the L^AT_EX file concerned, if the `achemso` package is not in use.

The style files are designed to use the `mciteplus` package if it is available, but to work even if it is not. When `mciteplus` is present, it is possible to automatically produce references of the form

(5) (a) Arduengo, A. J., III; Dias, H. V. R.; Harlow, R. L.; Kline, M. J. *Am. Chem. Soc.* **1992**, *114*, 5530–5534; (b) Appelhans, L. N.; Zuccaccia, D.; Kovacevic, A.; Chianese, A. R.; Miecznikowski, J. R.; Macchioni, A.; Clot, E.; Eisenstein, O.; Crabtree, R. H. *J. Am. Chem. Soc.* **2005**, *127*, 16299–16311; (c) Arduengo, A. J., III; Gamper, S. F.; Calabrese, J. C.; Davidson, F. *J. Am. Chem. Soc.* **1994**, *116*, 4391–4394.

as demonstrated in the example document. When `mciteplus` is not present, this functionality is not available but the style files will work normally.

The BibT_EX style files implement the bibliographic style specified by the ACS in *The ACS Style Guide*.² By default, article titles are not included in output using the `achemso.bst` file, but are with the `biochem.bst` file.

7 The natmove package

The `natmove` package does only one job. It brings the ability to move punctuation after citations, using code borrowed from the `cite` package. Both the `achemso` class and package load `natmove` automatically.

```
Some text \cite{Coghill2006} some more text.\\
Some text ending a sentence \cite{Coghill2006}.
Some text2 some more text.
Some text ending a sentence.2
```

This is deactivated for other citation types.

```
Some text \citeyear{Coghill2006}.\\
Some text \citeauthor{Coghill2006}.\\
Some text \citenum{Coghill2006}.
Some text 2006.
Some text Coghill and Garson.
Some text 2.
```

The package does nothing if the `super` option has not been given to `natbib`. This means that the source can be written without needing to decide where citations will to appear, with the `super` option for `natbib` controlling the result.

`\natmovechars`

One user macro is provided: `\natmovechars`. This contains the characters which are moved before superscript punctuation. The default contents is `,;:.` and can be set using `\renewcommand*`:

Some text², more text.²

```
\renewcommand*{\natmovechars}{.}  
Some text \cite{Coghill2006},  
more text \cite{Coghill2006}.
```


8 Change History

v1.0	General: Initial release of package by Mats Dahlgren 1	or remove dependency on other packages 1
v2.0	General: Re-write of package by Joseph Wright 1	Added \alsoaffiliation macro 3
v3.0	General: Second re-write, converting to a class and giving much tighter integration with ACS submission system 1	v3.2
v3.1	General: Re-ordered code to reduce	General: New functions \AbstractOff and \AbstractOn 5
		New functions \SectionsOff, \SectionsOn, \SectionNumbersOff and \SectionNumbersOn 5
		New tocentry section 5

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.

A	environments:	biochemistry 6
\AbstractOff 5	acknowledgement . . 5	journal 2
\AbstractOn 5	chart 5	manuscript 3
acknowledgement (environment) 5	graph 5	maxauthors 6
\affiliation 3	scheme 5	super 6
\alsoaffiliation 3	suppinfo 5	usetitle 6
\altaffiliation 3	tocentry 5	
\and 3		S
\author 3	G	scheme (environment) . . 5
	graph (environment) . . . 5	\SectionNumbersOff . . 5
B		\SectionNumbersOn . . . 5
biblabel (option) 6	J	\SectionsOff 5
\bibnote 6	journal (option) 2	\SectionsOn 5
\bibnotemark 6		super (option) 6
\bibnotetext 6	M	suppinfo (environment) 5
biochem (option) 6	manuscript (option) . . . 3	
biochemistry (option) . 6	maxauthors (option) . . . 6	T
	N	\thanks 3
C	\natmovechars 7	tocentry (environment) 5
chart (environment) . . . 5	O	
	options:	U
E	biblabel 6	usetitle (option) 6
\email 3	biochem 6	

10 References

[1] This note text will be in the bibliography.

- [2] *The ACS Style Guide*, 3rd ed.; Coghill, A. M., Garson, L. R., Eds.; Oxford University Press, Inc. and The American Chemical Society: New York, 2006.