

# achemso — Support for submissions to American Chemical Society journals\*

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## Abstract

The `achemso` bundle provides a  $\text{\LaTeX}$  class file and  $\text{\BibTeX}$  style file in accordance with the requirements of the American Chemical Society. 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  $\text{\BibTeX}$  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.

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

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\*This file describes version v3.1a, last revised 2009/02/03.

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changes to facilitate ease of use. The second part is the L<sup>A</sup>T<sub>E</sub>X package, which is loaded by the class. The package contains the parts of the bundle which might be appropriate for use with other document classes.<sup>1</sup> Thirdly, two B<sub>I</sub>B<sub>T</sub>E<sub>X</sub> 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 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.

### 2.1 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 Table 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.

### 2.2 Manuscript meta-data

`\title` When using the `achemso` class, the `\title` macro takes an optional argument. This is intended for a short version of the title, for use in running headers. The title in the running headers is designed to ensure that print-outs of the manuscript are easily identified.

`\author` Inspired by REV<sub>T</sub>E<sub>X</sub>4, the `achemso` class alters the method for adding author information to the manuscript. Each author should be given as a separate `\affiliation` 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.<sup>2</sup> At least one author should be

<sup>1</sup>For example, when writing a thesis.

<sup>2</sup>This will usually be the university or company name.

Table 1: Values for journal option

<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

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`  
`\thanks` and `\thanks` macros are not appropriate in the `achemso` class. Both produce a warning if used.

The meta-data items should be given in the preamble to the  $\LaTeX$  file, and no `\maketitle` macro is required in the document body. This is all handled by the class file directly. At least one author, affiliation and e-mail address must be specified.

## 2.3 Bibliography notes

`\bibnote` By loading the `notes2bib` package, the class provides the `\bibnote` 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  $\BibTeX$ .

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

## 2.4 Floats

`scheme`      The class defines three new floating environments: `scheme`, `chart` and `graph`.<sup>3</sup>  
`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.

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<sup>3</sup>This is done in the class as life is complex for packages due to differing mechanisms in `memoir` and `KOMA-script`.

## 2.5 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 JACS 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}
```

## 3 The package file

The package file is loaded by the class, but can also be loaded independently. The class contains only items focussed on submission; more generally-useful items are stored in the package.

### 3.1 Altering the behaviour of natbib

achemso comes with the natmove package, which adds cite-like functionality to natbib.<sup>4</sup> Thus citations may be made using all of the natbib commands (`\citeauthor`, `\citeyear`, *etc.*). For superscript citations, the number will be moved after punctuation as needed. The user should therefore write citations suitable for “in line” use and leave the positioning to the package.

Some text<sup>2</sup> some more text.  
Some text ending a sentence.<sup>2</sup>

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

### 3.2 Package options

The `journal` and `manuscript` options have no effect when using the package without the class. Instead, the user can control various aspects of the behaviour of the package directly.<sup>5</sup> The options all relate to aspects of reference handling.

super The `super` option affects the handling of superscript reference markers. The option switches this behaviour on and off (and takes Boolean values: `super=true` and `super=false` are valid).

maxauthors The `maxauthors` and `usetitle` options change the output of the BibTeX style files. `maxauthors` 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 `usetitle` option is a Boolean, and sets whether the title of a paper referenced appears in the bibliography. The default is `usetitle=false`.

biblabe The `Redefining the formatting of the numbers used in the bibliography usually re-`

<sup>4</sup>The code is a copy from cite with minor modifications.

<sup>5</sup>Using the package alone probably means a report or thesis is being written, and so prescriptive application of journal style is not appropriate.

biochemistry  
 biochem

quires modifying internal L<sup>A</sup>T<sub>E</sub>X macros. The `biblabel` option makes these changes more accessible: valid values are `plain` (use the number only), `brackets` (surround the number in brackets) and `period or fullstop` (follow the number by a full stop/period).

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 *Biochemistry* is probably the most prominent. The `biochemistry` or `biochem` option uses the style of *Biochemistry* for the bibliography, rather than the normal ACS style. For this style, the `usetitle=true` option is the default.<sup>6</sup>

## 4 The BibT<sub>E</sub>X 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` and `mictplus` packages must be loaded by the L<sup>A</sup>T<sub>E</sub>X file concerned, if the `achemso` package is not in use.

The BibT<sub>E</sub>X style files implement the bibliographic style specified by the ACS in *The ACS Style Guide*.<sup>2</sup> By default, article titles are not included in output using the `achemso.bst` file, but are with the `biochem.bst` file.

## 5 Change History

2008/11/08		v2.0	
General: Added <code>\alsoaffiliation</code> macro	..... 2	General: Re-write of package by Joseph Wright	..... 1
		v3.0	
v1.0		General: Second re-write, converting to a class and giving much tighter integration with ACS submission system	..... 1
General: Initial release of package by Mats Dahlgren	..... 1		

## 6 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		\author	
acknowledgement (environment)	... 5		2
\affiliation	..... 2	B	
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\altaffiliation	..... 2	<code>\bibnote</code>	4
\and	..... 4	<code>biochem</code> (option)	6

<sup>6</sup>More accurately, the default built into the BibT<sub>E</sub>X style file is to use article titles with the *Biochemistry* style.

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		<b>U</b>	
		usetitle (option) .....	5

## 7 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.