

# 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 (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  $\text{\BibTeX}$  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.

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\*This file describes version v3.7f, last revised 2013/07/07.

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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  $\text{\LaTeX}$  package. The package contains the parts of the bundle which are appropriate for use with other document classes.<sup>1</sup> Thirdly, two  $\text{\BibTeX}$  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 package is supplied in dtx format and as a pre-extracted zip file, `achemso.tds.zip`. The later is most convenient for most users: simply unzip this in your local texmf directory and run `texhash` to update the database of file locations. If you want to unpack the dtx yourself, running `tex chemso.dtx` will extract the package whereas `latex chemso.dtx` will extract it and also typeset the documentation.

Typesetting the documentation requires a number of packages in addition to those needed to use the package. This is mainly because of the number of demonstration items included in the text. To compile the documentation without error, you will need the packages:

- array
- booktabs
- hypdoc
- listings
- lmodern
- mathpazo
- microtype

## 3 Requirements

The `achemso` class requires the following packages:

- caption
- float
- geometry
- natbib
- setspace
- xkeyval

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

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

## 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.

### 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.
- `layout` The `achemso` class can produce drafts in two layout styles. The standard setting for the `layout` option is `traditional`, which produces a double-spaced single column manuscript. The alternative setting `twocolumn` will use single spacing and print the text in two columns. The second option is obviously more compact. If the journal requires a particular style this option may be ignored.
- `email` It may be desirable to omit e-mail addresses from the front page of a manuscript. The printing of e-mail addresses can be disabled using the `email` option, which takes Boolean values only. The default is to print e-mail addresses. Notice that phone and fax numbers are only printed if e-mail addresses are printed.

Other options are provided by the package, but when used with the class these are silently ignored. If you need to override the settings chosen by the class, include the settings *after* the `\documentclass` line using `\setkeys`:

```
\documentclass[journal = jacsat]{achemso}
\setkeys{acs}{articletitle = true}
```

### 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.<sup>2</sup> At least one author should be followed by an
- `\alsoaffiliation`
- `\altaffiliation`
- `\email`

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

<i>Journal</i>	<i>Setting</i>
<i>ACS Chem. Biol.</i>	acbcct
<i>ACS Catal.</i>	accacs
<i>Acc. Chem. Res.</i>	achre4
<i>ACS Chem. Neurosci.</i>	acncdm
<i>ACS Combinatorial Sci.</i>	acsccc
<i>ACS Med. Chem. Lett.</i>	amclct
<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. Ed.</i>	jceda8
<i>J. Chem. Inf. Model.</i>	jcisd8
<i>J. Chem. Theory Comput.</i>	jctcce
<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. Phys. Chem. Lett.</i>	jpclcd
<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

\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}
```

Repeated entries for \affiliation and \alsoaffiliation will result in only one address being printed in the address list and footnotes. Repeated \altaffiliation entries only produce a single footnote, and can therefore be used for entries such as

```
\author{First Coworker}
\altaffiliation{Contributed equally to this work}
\author{Second Coworker}
\altaffiliation{Contributed equally to this work}
```

if required.

\fax           The class will recognise the optional information \fax and \phone, which  
\phone       will be printed along with the lead authors e-mail address. Note that this  
              information is only used for authors who have an e-mail address supplied.

```
\author{Second Bloke}
\email{second.bloke@some.place}
\phone{+xxx (0)yyy zzzzzz}
\fax{+xxx (0)yyy wwwwww}
\affiliation[University of Sometown]
    {University of Somewhere, Sometown, USA}
```

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

\title        The \title macro is extended to accept an optional argument. This is  
              intended for a shortened version of the journal title suitable for running headers.  
              Some journals require that authors supply this data: if it is needed then it will be  
              printed in the appropriate place.

```
\title[Short running title]
    {Long title which would not fit in running headers}
```

The meta-data items should be given in the preamble to the L<sup>A</sup>T<sub>E</sub>X 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.

### 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.

### 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`  
`\AbstractOff` macros, which again are preamble-only. Similar functions are available for the  
`\AbstractOn` abstract: `\AbstractOff` and `\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{acknowledgement}
  The authors thank A.N.-Other.
\end{acknowledgement}

\begin{suppinfo}
  Full characterization data for all new compounds.
\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!

- `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).
- `articletitle` The `articletitle` option is a Boolean, and sets whether the title of a paper referenced appears in the bibliography. The default is `articletitle=false` for the `achemso` style and `articletitle=true` for the `biochem` style.
- `chaptertitle` The option boolean `chaptertitle` option is provided to allow flexibility for the inclusion of chapter titles for book and related entries. The standard setting is `false`: setting it to `true` will cause chapter titles to be included.
- `etalmode` Many journals require that long lists of authors are shortened using ‘et al.’ in the references section. The behaviour of the `BibTeX` styles in this regard is controlled by two options, `etalmode` and `maxauthors`. There are two possible ways to shorten a long list of authors. Some journals require that only the first author is given, followed by ‘et al.’: for this behaviour, set `etalmode=firstonly`:

Jones, A.N. et al.

On the other hand, some journals request that the list of authors is truncated after  $n$  authors. This is set up by the `etalmode=truncate` option:

Jones, A.N.; Bloggs, F.; Nobacon, D. et al.

In both cases, the maximum number of authors permitted before introducing ‘et al.’ is governed by the `maxauthors` option. This option recognises the sentinel value 0, which indicates that no shortening should occur at all.

- `biblabel` Redefining the formatting of the numbers used in the bibliography usually requires modifying internal `LaTeX` 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).
- `biochem` 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 `articletitle=true` option is the default.<sup>3</sup>
- `biochemistry`

## 5.2 Bibliography notes

- `\bibnote` `achemso` 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`. In analogy to `\footnote`, the macros `\bibnotemark` and `\bibnotetext` are available for dividing up the marker for a note from the text.

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

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

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.

## 6 The Bib<sub>T</sub><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` package must be loaded by the  $\LaTeX$  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 Bib<sub>T</sub><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.

The style used by the ACS does not differentiate between Bib<sub>T</sub><sub>E</sub>X `book`, `inbook`, `collection` and `incollection` entries. As a result, the appearance of these entry types depends on the fields available. Named subdivisions of a book (for example, chapters where each has a named author) should be given in the `title` field, with the title of the book itself in the `booktitle` field. The `chapter` field should be used for a chapter number, and is printed as part of the pagination.

One frequently asked question is why some people see an empty first item in their bibliography when using the `achemso` package or class. This is usually because they have downloaded the  $\LaTeX$  files and done a local installation without also updating the Bib<sub>T</sub><sub>E</sub>X style. The two must be from the same version of `achemso`: they are designed to work together.

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

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 text<sup>2</sup>, more text.<sup>2</sup> `\renewcommand*{\natmovechars}{.}`  
Some text `\cite{Coghill2006}`,  
more text `\cite{Coghill2006}`.

## 8 Change History

v1.0	General: Initial release of package by Mats Dahlgren . . . . . 1	v3.2b	General: New email option . . . . . 3
v2.0	General: Re-write of package by Joseph Wright . . . . . 1	v3.2c	General: Added <code>\fax</code> macro . . . . . 5 Added <code>\phone</code> macro . . . . . 5 Fix so that email option is turned on by default . . . . . 3
v3.0	General: Second re-write, converting to a class and giving much tighter integration with ACS submission system . . . . . 1	v3.3	General: <code>\altaffiliation</code> macro checks for duplicate entries and uses only one footnote . . . . . 3 New layout option . . . . . 3
v3.1	General: Re-ordered code to reduce or remove dependency on other packages . . . . . 1 Added <code>\alsoaffiliation</code> macro . . . . . 3	v3.3a	General: New <code>etalmode</code> option . . . 7
v3.2	General: New functions <code>\AbstractOff</code> and <code>\AbstractOn</code> . . . . . 6 New functions <code>\SectionsOff</code> , <code>\SectionsOn</code> , <code>\SectionNumbersOff</code> and <code>\SectionNumbersOn</code> . . . . . 6 New <code>tocentry</code> section . . . . . 6	v3.4	General: More detail on installation Require <code>cleveref</code> , dropping <code>varioref</code> use . . . . . 2
		v3.5	General: New BibTeX style file. . . . 1
		v3.5a	General: Modify JACS Communication to print abstract . . . . . 1
		v3.5c	General: Bug fix for <code>\mciteSubRef</code>

macro	..... 1	v3.7	
Update <i>Org. Lett.</i> style	..... 1		General: New <code>chaptertitle</code> option for bibliography ..... 7
v3.6			Rename <code>usetitle</code> option to <code>articletitle</code> ..... 7
General: Drop <code>cleverref</code> use	..... 2		

## 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.

<b>A</b>		chart ..... 6	biochem ..... 7
\AbstractOff ..... 6	graph ..... 6	biochemistry ..... 7	
\AbstractOn ..... 6	scheme ..... 6	chaptertitle ..... 7	
acknowledgement (environment) ..... 6	suppinfo ..... 6	email ..... 3	
	tocentry ..... 6	etalmode ..... 7	
\affiliation ..... 3	etalmode (option) ..... 7	journal ..... 3	
\alsoaffiliation ..... 3		layout ..... 3	
\altaffiliation ..... 3	<b>F</b>	manuscript ..... 3	
\and ..... 5	\fax ..... 5	maxauthors ..... 7	
articletitle (option) . 7		super ..... 7	
\author ..... 3	<b>G</b>		
	graph (environment) ... 6	<b>P</b>	
<b>B</b>		\phone ..... 5	
biblabel (option) ..... 7	<b>J</b>		
\bibnote ..... 7	journal (option) ..... 3	<b>S</b>	
\bibnotemark ..... 7		scheme (environment) .. 6	
\bibnotetext ..... 7	<b>L</b>	\SectionNumbersOff .. 6	
biochem (option) ..... 7	layout (option) ..... 3	\SectionNumbersOn ... 6	
biochemistry (option) . 7	<b>M</b>	\SectionsOff ..... 6	
	manuscript (option) ... 3	\SectionsOn ..... 6	
	maxauthors (option) ... 7	super (option) ..... 7	
<b>C</b>		suppinfo (environment) ..... 6	
chaptertitle (option) . 7	<b>N</b>		
chart (environment) ... 6	\natmovechars ..... 9	<b>T</b>	
<b>E</b>			
\email ..... 3	<b>O</b>	\thanks ..... 5	
email (option) ..... 3	options:	\title ..... 5	
environments:	articletitle ..... 7	tocentry (environment) ..... 6	
acknowledgement .. 6	biblabel ..... 7		

## 10 References

- [1] This note text will be in the bibliography.
- [2] Coghill, A. M., Garson, L. R., Eds. *The ACS Style Guide*, 3rd ed.; Oxford University Press, Inc. and The American Chemical Society: New York, 2006.