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 BtbTeX 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.

^{*}This file describes version v3.9a, last revised 2015/03/12.

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The bundle consists of four parts. The first is a LATEX 2ε 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. 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 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 achemso.dtx will extract the package whereas latex achemso.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
- Imodern
- mathpazo
- microtype

3 Requirements

The achemso class requires the following packages:

- caption
- float
- geometery
- natbib
- setspace
- xkeyval

These are normally present in the current major TEX distributions, but are also available from The Comprehensive TeX Archive Network.

¹For example, when writing a thesis.

Journal	Setting	Journal	Setting
ACS Appl. Mater. Interfaces	aamick	Ind. Eng. Chem. Res.	iecred
ACS Chem. Biol.	acbcct	Inorg. Chem.	inoraj
ACS Catal.	accacs	J. Agric. Food Chem.	jafcau
ACS Central Sci.	acscii	J. Chem. Eng. Data	jceaax
Acc. Chem. Res.	achre4	J. Chem. Ed.	jceda8
ACS Chem. Neurosci.	acncdm	J. Chem. Inf. Model.	jcisd8
ACS Combinatorial Sci.	acsccc	J. Chem. Theory Comput.	jctcce
ACS Macro Lett.	amlccd	J. Med. Chem.	jmcmar
ACS Med. Chem. Lett.	amclct	J. Nat. Prod.	jnprdf
ACS Nano	ancac3	J. Org. Chem.	joceah
ACS Photon.	apchd5	J. Phys. Chem. A	jpcafh
ACS Sustainable Chem. Eng.	ascecg	J. Phys. Chem. B	jpcbfk
ACS Synth. Biol.	asbcd6	J. Phys. Chem. C	jpccck
Anal. Chem.	ancham	J. Phys. Chem. Lett.	jpclcd
Biochemistry	bichaw	J. Proteome Res.	jprobs
Bioconjugate Chem.	bcches	J. Am. Chem. Soc.	jacsat
Biomacromolecules	bomaf6	Langmuir	langd5
Chem. Res. Toxicol.	crtoec	Macromolecules	mamobx
Chem. Rev.	chreay	Mol. Pharm.	mpohbp
Chem. Mater.	cmatex	Nano Lett.	nalefd
Cryst. Growth Des.	cgdefu	Org. Lett.	orlef7
Energy Fuels	enfuem	Org. Proc. Res. Dev.	oprdfk
Environ. Sci. Technol.	esthag	Organometallics	orgnd7
Environ. Sci. Technol. Lett.	estlcu	-	

Table 1: Values for journal option

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 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.

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, inlcude the settings *after* the \documentclass line using \setkeys:

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

4.2 Manuscript meta-data

\author \affiliation \alsoaffiliation \altaffiliation \email 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. 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}
```

²This will usually be the university or company name.

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 \phone The class will recognise the optional information \fax and \phone, which 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 \thanks 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.

\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 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.

4.3 Floats

scheme chart graph The class defines three new floating environments: scheme, chart and graph. These can be used as expected to include graphical content. The placement of 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 \SectionNumbersOn Some journals have no section numbering by default. This can be set up in 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 \SectionsOn More radically, the entire availability of sections can be turned on and of. This is functionality is available to the user via the \SectionsOn and \SectionsOff

\AbstractOff
\AbstractOn

macros, which again are preamble-only. Similar functions are available for the abstract: \AbstractOff and \AbstractOn.

4.5 Special sections

acknowledgement suppinfo

The sections for acknowledgements and supporting information have dedicated 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}
```

4.6 Miscellaneous commands

\latin

The command \latin is provided by the class to format Latin phrases such as "et al." Most ACS journals do not make these italic, but some (for example ACS Nano) do. By providing a command, the formatting is left flexible.

5 The package file

The achemso package is independent of the classs 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.

doi

The boolean doi option is provided to allow a DOI (Digital Object Identifier) to be included for bibliography entries even where other identification such as page numbers is available. The standard setting is false: setting it to true will cause DOI numbers to be printed if available.

chaptertitle

The 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 maxauthors

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 biochemistry

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.³

5.2 Bibliography notes

\bibnote \bibnotemark \bibnotetext 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.

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.

 $^{^3}$ More 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 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 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.

The style used by the ACS does not differentiate between BIBTEX 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 BibTEX 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*:

```
\renewcommand*{\natmovechars}{.}
Some text^2, more text.^2
Some text \cite{Coghill2006},
more text \cite{Coghill2006}.
```

8 Change History

V1.0	v3.5
General: Initial release of package	General: New BibT _E X style file 1
by Mats Dahlgren 1	v3.5a General: Modify JACS Communica-
General: Re-write of package by	tion to print abstract
Joseph Wright 1	V3.5C
V3.0	General: Bug fix for \mciteSubRef
General: 1	macro 1
V3.1	Update Org. Lett. style 1
General: 1	v3.6
Added \alsoaffiliation	General: Drop cleverref use 1
macro 1	V3.7
v3.2	General: New chaptertitle option for bibliography
General: 1	Rename usetitle option to
1	articletitle 1
New tocentry section 1	v3.8
V3.2b	General: Extend journal list to cur-
General: New email option 1	rent ACS range 1
v3.2c General: Added \fax macro 1	Introduce \latin command to
Added \phone macro 1	support ACS Nano requirements 1
Fix so that email option is turned	v3.8a
on by default 1	General: Minor style improvements for some journals
V3.3	v3.8b
General: \altaffiliation macro	General: Improve output ordering
checks for duplicate entries and	for J. Phys. Chem. Lett 1
uses only one footnote 1	v3.8c
New layout option 1	General: Improve ACS Photonics
v3.3a	style
General: New etalmode option 1	v3.8d
V3.4	General: Fix bug in keyword print-
General: More detail on installation 1	ing
Require cleveref, dropping varioref use	v3.8e General: Minor style changes for
usc 1	Octicial. Willion Style Changes 101

```
J. Med. Chem.
                        and ACS
                                            Update article title requirements
      Appl. Mater. . . . . . . . . . . . . . . 1
                                             for all journals ..... 1
                                            Update keyword requirements for
v3.8g
                                             General: Fix issue with J. Phys. Chem.
                                      v3.8k
      formatting ..... 1
                                          General: Format date correctly for
v3.8i
                                             in press bibliography entries ... 1
   General: Fix issue with Chem. Res.
                                      v3.81
      Toxicol. formatting . . . . . . . . . . 1
                                          General: Fix printing of phone/fax
v3.8j
                                             numbers \dots \dots 1
   General: Remove Biotechnol. Prog.
      configuration ..... 1
                                          General: New doi option . . . . . . . 1
```

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.

Α	environments:	biblabel 7
\AbstractOff 6	acknowledgement 6	biochem 7
\AbstractOn 6	chart 5	biochemistry 7
acknowledgement (envi-	graph 5	chaptertitle 7
ronment) 6	scheme5	doi 7
\affiliation 4	suppinfo \dots 6	email 4
\alsoaffiliation 4	tocentry 6	etalmode 7
\altaffiliation 4	etalmode (option) 7	journal 3
\and 5	_	layout 4
articletitle (option) . 6	F	manuscript 4
\author 4	\fax 5	maxauthors 7
•	G	super 6
В	graph (environment) 5	n.
biblabel (option) 7	gruph (environment) y	P
\bibnote 7	J	\phone 5
\bibnotemark 7	journal (option) 3	S
\bibnotetext 7		scheme (environment) 5
biochem (option) 7	L	\SectionNumbersOff 5
biochemistry (option) . 7	\latin 6	\SectionNumbersOn 5
•	layout (option) 4	\SectionsOff5
C	М	\SectionsOn5
chaptertitle (option) . 7	manuscript (option) 4	super (option) 6
chart (environment) 5	maxauthors (option) 7	suppinfo (environ-
	maxauthors (option) /	ment) 6
D	N	,
doi (option) 7	\natmovechars 9	T
		\thanks 5
E	О	\title 5
\email 4		tocentry (environ-
email (option) 4		ment) 6

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.