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. 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.

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, which is

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loaded by the class. The package contains the parts of the bundle which might be appropriate for use with other document classes. Thirdly, two BibT_EX 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.

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 \affiliation \altaffiliation \email Inspired by REVTeX4, 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.

¹For example, when writing a thesis.

²This will usually be the university or company name.

Table 1: Values for journal option

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

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

\and \thanks The method used for setting the meta-data means that the normal \and \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. 1

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

2.4 Floats

scheme chart graph The class defines three new floating environments: scheme, chart and graph.³ 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.

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.

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.⁴ Thus citations may be made using all of the natbib commands

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

⁴The code is a copy from cite with minor modifications.

(\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 text² some more text. Some text ending a sentence.²

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.⁵ 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 usetitle

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 o 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.

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).

biochemistry 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 usetitle=true option is the default.⁶

4 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 and micteplus packages must be loaded by the LATEX file concerned, if the achemso package is not in use.

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

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

⁶More accurately, the default built into the BibT_EX style file is to use article titles with the *Biochemistry* style.

5 Change History

| V1.0 | V3.0 | |
|-------------------------------------|------------------------------------|--|
| General: Initial release of package | | |
| by Mats Dahlgren 1 | General: Second re-write, convert- | |
| V2.0 | ing to a class and giving much | |
| General: Re-write of package by | tighter integration with ACS sub- | |
| Joseph Wright 1 | mission system 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.

| ${f A}$ | M |
|---|------------------------|
| \affiliation 2 | manuscript (option) 2 |
| \altaffiliation 2 | maxauthors (option) 5 |
| \and 4 | |
| \author 2 | O |
| B biblabel (option) 5 \bibnote 4 biochem (option) 5 biochemistry (option) 5 | journal 2 manuscript 2 |
| C | maxauthors 5 |
| chart (environment) 4 | |
| E | usetitle 5 |
| \email | scheme (environment) 4 |
| G graph (environment) | \thanks 4 |
| J journal (option) 2 | U 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.