achemso— LaTeX and BibTeX support for American Chemical Society publications*

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Abstract

The achemso package provides a BibTeX style in accordance with the requirements of the journals of the American Chemical Society, along with a supporting LaTeX package file. Also provided are a number of BibTeX style files to be used for bibliography database listings, including support for natbib and mciteplus.

1 Introduction

Synthetic chemists do not, in the main, use LaTeX for the preparation of journal articles. Some journals, mainly in the physical chemistry area, do accept LaTeX submissions. Given the clear advantages of LaTeX over other methods, it would be nice to be able to use LaTeX for preparing reports. Thus the need for BibTeX styles for chemistry is real. The package achemso provides for a BibTeX style and other support for articles and reports in the style of the American Chemical Society (ACS).

As describe in *The ACS Style Guide*,[1] almost all ACS publications use the same style for the formatting of references. The reproduction of this style is the aim of the BibTeX style file provided here. However, the ACS use different citation styles in different publications. The achemso package provides support for the two numerical systems: superscript and italic in-text citations. The majority of ACS journals use the superscript method (Table 1), with a smaller number using the italic system (Table 2). The journal *Biochemistry* does not use the standard ACS style for references, and so is not covered by the achemso package. The journal *Industrial & Engineering Chemistry Research* uses a modification of the standard ACS style; it is covered by achemso using the `iecr.bst` files and derivatives.

This package consists of a number of BibTeX files along with a small LaTeX file `achemso.sty`. The naming of the package is slightly unusual, but follows from the need to pick a unique name. To quote the documentation to the first version:

> there is already a LaTeX 2.09 and BibTeX style package called acsarticle and `acs.bst`, which are not "ACS" as in 'American Chemical Society' (rather, this package is formatting the output according to the

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Table 1: Journals using the ACS reference style with superscript citations

Journal Title	*CASSI* Abbreviation
Accounts of Chemical Research	*Acc. Chem. Res.*
Analytical Chemistry	*Anal. Chem.*
Biomacromolecules	*Biomacromolecules*
Chemical Reviews	*Chem. Rev.*
Chemistry of Materials	*Chem. Mater.*
Crystal Growth & Design	*Cryst. Growth Des.*
Energy & Fuels	*Energy Fuels*
Industrial & Engineering Chemistry Research	*Ind. Eng. Chem. Res.*
Inorganic Chemistry	*Inorg.Chem.*
Journal of the American Chemical Society	*J. Am. Chem. Soc.*
Journal of Chemical and Engineering Data	*J. Chem. Eng. Data*
Journal of Chemical Theory and Computation	*J. Chem. Theory Comput.*
Journal of Chemical Information and Modeling	*J. Chem. Inf. Model.*
Journal of Combinatorial Chemistry	*J. Comb. Chem.*
Journal of Medicinal Chemistry	*J. Med. Chem.*
Journal of Natural Products	*J. Nat. Prod.*
The Journal of Organic Chemistry	*J. Org. Chem.*
The Journal of Physical Chemistry A	*J. Phys. Chem. A*
The Journal of Physical Chemistry B	*J. Phys. Chem. B*
The Journal of Physical Chemistry C	*J. Phys. Chem. C*
Journal of Proteome Research	*J. Proteome Res.*
Langmuir	*Langmuir*
Macromolecules	*Macromolecules*
Molecular Pharmaceutics	*Mol. Pharm.*
Nano Letters	*Nano Lett.*
Organic Letters	*Org. Lett.*
Organic Process Research & Design	*Org. Process Res. Dev.*
Organometallics	*Organometallics*

Table 2: Journals using the ACS reference style with in-text citations

Journal Title	*CASSI* Abbreviation
ACS Chemical Biology	*ACS Chem. Biol.*
Bioconjugate Chemistry	*Bioconjugate Chem.*
Biotechnology Progress	*Biotechnol. Prog.*
Chemical Research in Toxicology	*Chem. Res. Toxicol.*
Environmental Science and Technology	*Envirn. Sci. Technol.*
Journal of Agricultural and Food Chemistry	*J. Agric. Food Chem.*

instructions of *Advances in Control Systems*). Hence, *this* new package had to be given another name. The name of choice was then achemso, which is made from the words "*A*merican *Chem*ical *So*ciety."

1.1 Change of maintainer

This package was initially released by Mats Dahlgren. He no longer has time to devote to LaTeX development. With his permission, the package has therefore been taken over by Joseph Wright, the maintainer of the the rsc package. The majority of the package has been rebuilt and the BibTeX style file has been totally overhauled. Any mistakes are entirely the fault of the new maintainer!

2 The BibTeX style files

The BibTeX style files implement the bibliographic style specified by the ACS in *The ACS Style Guide*,[1] on the ACS website,[2] and in current ACS publications. Some of this information can be contradictory, and *The ACS Style Guide* sometimes gives more than one option as a model. In order to resolve cases where several possibilities are available current editions of the *Journal of the American Chemical Society* have been consulted; the current consensus there has been taken as the correct approach. In addition to the problem of picking the correct style, some of the BibTeX record types are difficult to match to standard references in ACS journals. The "best guess" has been taken with these.

2.1 Additional record types

In general, the database record types supported here follow those in the standard BibTeX style files. Four additional record types are provided:

patent A patent: formatting is similar to other record types. The data entry for this record type follows the pattern used in `rsc.bst`: `journal` is used to hold the patent type (*e.g.*. "U.S. Patent"), with the patent number given in `pages`. Whilst this format is non-standard, it is relatively easy to use and implement!

submitted Articles submitted to journals but not yet accepted: appends "submitted" in a suitable fashion to the entry.

inpress Articles in press: appends "in press" or, if available, the DOI number assigned to the article.

remark A note with no other information to be included. Output consists purely of the `note` field.

2.2 BibTeX database entry requirements

The requirements for entries in the BibTeX database are slightly different using `achemso.bst` to the standard style files. This is mainly because some fields are not cited in ACS bibliographies. In particular, journal articles do not require a title (the `title` field is ignored). Articles in books and "collections" only need

the title of the book. If a chapter title is given for an `incollection` record, it will be printed, but not in the case of an `inbook` record.

2.3 References to software

Referencing software is always a little difficult. The style files provided here follow the normal LaTeX convention of using the `manual` record type to cite software. The only requirement is a `title`, but fields such as `organization` may be used for more detail. The `edition` field is used to format the software version correctly: this will automatically be prefixed with "version" by the style file.

2.4 The `annotate` field

The standard BibTeX styles use the `note` field for notes to be added to the citation. However, it is common to want personal notes about references. This is catered for using the `annotate` field. The style `achemso` ignores the `annotate` field, whilst the `achemsol` style appends the `annotate` information to the bibliographic output. Thus `achemsol` is intended for use in database maintenance, whilst `achemso` is for production bibliographies.

`\refin` For use in the `annotate` field the macro `\refin` is defined in `achemso.bst` and `achemsol.bst`. The command takes a single argument `{`⟨*text*⟩`}`, and gives the output **Referenced in: text**. This command takes one argument (normally text) which is preceded by the text "**Referenced in:** ⟨*text*⟩". The `\refin` command is intended for tracking citations "backward" through the database. For example, this could be used to link citations in a database to the writer's own papers.

2.5 Predefined journal abbreviations

A number of journal abbreviations are defined in the `.bst` files. The abbreviations cover a number ACS journals, several other physical chemistry publications and other journals listed as highly cited by *Chem. Abs.* The interested user should consult the `.bst` files for full details.

2.6 Multiple citations: mciteplus support

By default, BibTeX does not handle producing compound references. The mciteplus package solves this problem, and is highly recommended to users of achemso. This allows you to put something like:

```
\documentclass{article}
\usepackage{mciteplus}
\begin{document}
\cite{Wanzlick1962,*Ofele1968}
\bibliography{example}
\bibliographystyle{achemsoM}
\end{document}
```

and get output of the form:

1. (a) Wanzlick, H. W. *Angew. Chem., Int. Ed. Engl.* **1962**, *1*, 75–80; (b) Öfele, K. *J. Organomet. Chem.* **1968**, *12*, P42–P43.

in the bibliography. Notice the change of `\bibliographystyle` from `achemso` to `achemsoM`.

2.7 natbib support

As of version 2.2, a natbib compatible style file, `achemnat` is provided. The style file provides the appropriate option, natbib, to load this BibTeX file along with natbib, setting up the appropriate options.

3 The LaTeX Package

The current version of `achemso.sty` is a complete re-implementation of the functionality of the original file, designed to ensure greater compatibility with other packages. The only change for the user is that the bibliography section does *not* start a new page when using the `article` document class. However, the package now supports all of the standard classes, and so the `report` class may be used to ensure a new page is started.

`\bibliographystyle` Loading the achemso package adds the appropriate `\bibliographystyle` command to the LaTeX source. As a result, subsequent `\bibliographystyle` statements will be ignored: a suitable warning is given. The format of citations is altered (using the cite or natbib package as appropriate), and the package ensures that the bibliography will be named "References" in all standard document types.[1]

The achemso package has options:

note If the bibliography contains notes as well as citations, then the section heading should be "References and Notes". This is altered by the `note` package option.

number This option numbers the bibliography section (using the tocbibind package), and causes it to be entered in the Table of Contents.

list This option is intended for creating a listing of the entire BibTeX database. The BibTeX style is changed to achemso, which will output the additional database field `annotate`, intended for personal notes about a particular database entry. It also adds the BibTeX key for each citation as a marginal note to the output, using the showkeys package.

notsuper Switches from superscript citations (*e.g.*. Author *et al.*[3]) to in-text ones in italics (*e.g.*. Author *et al.* (3)). There is a `super` option for completeness, which simply gives the default behaviour.

natbib Uses natbib rather than cite for citation formatting; this also loads the `achemnat` style in place of `achemso`.

mcite Uses the mciteplus-compatible version of the BibTeX style file, and loads mciteplus.

[1] This only works if the babel package is *not* loaded. Users wanting a system which works with babel should look at the chemstyle package.

iecr Uses a setup suitable for the journal *Industrial & Engineering Chemical Research*.

usetitle Adds journal titles in bibliography (equivalent to `iecr` option).

4 The Package Code

The package code is not very complicated. For the interested reader(s), it is presented here. The usual setup code is executed.

```
⟨*package⟩
\NeedsTeXFormat{LaTeX2e}
\ProvidesPackage{achemso}
  [2008/04/16 v2.2i LaTeX and BibTeX support for American
     Chemical Society publications]
```

\ifACS@sctnnmbr
\ifACS@list
\ifACS@note
\ifACS@super
\ifACS@natbib
\ifACS@mcite
\ifACS@iecr

Boolean values are used to handle the options.

```
\newif\ifACS@sctnnmbr\ACS@sctnnmbrfalse
\newif\ifACS@list\ACS@listfalse
\newif\ifACS@note\ACS@notefalse
\newif\ifACS@super\ACS@supertrue
\newif\ifACS@natbib\ACS@natbibfalse
\newif\ifACS@mcite\ACS@mcitefalse
\newif\ifACS@iecr\ACS@iecrfalse
```

The options are processed.

```
\DeclareOption{note}{\ExecuteOptions{notes}}
\DeclareOption{notes}{\ACS@notetrue}
\DeclareOption{number}{\ACS@sctnnmbrtrue}
\DeclareOption{super}{\ACS@supertrue}
\DeclareOption{list}{\ACS@listtrue}
\DeclareOption{notsuper}{\ACS@superfalse}
\DeclareOption{natbib}{\ACS@natbibtrue}
\DeclareOption{mcite}{\ACS@mcitetrue}
\DeclareOption{iecr}{\ACS@iecrtrue}
\DeclareOption{usetitle}{\ACS@iecrtrue}
\DeclareOption*{\OptionNotUsed}
\ProcessOptions\relax
```

The cite package is loaded to sort and compress references correctly. Depending upon the package option given, citations are either superscript or italic and in parentheses.

```
\ifACS@natbib
  \ifACS@super
    \RequirePackage[numbers,sort&compress,super]{natbib}
  \else
```

\citenumfont

For in-line citations with natbib, we have to do a bit of work to get things to look right. natbib uses `\citenumfont` to format the numbers, but it is not defined by default, so we have to use `\newcommand`.

```
    \RequirePackage[numbers,sort&compress,round]{natbib}
    \newcommand*{\citenumfont}{\textit}
  \fi
```

```
\else
  \ifACS@super

    \RequirePackage[nospace]{overcite}
  \else
```

Again in-line citations need some format changes. In the case of cite, everything is defined initially. Thus we can use `\renewcommand` for everything.

```
    \RequirePackage{cite}
    \renewcommand{\citeleft}{(}
    \renewcommand{\citeright}{)}
    \renewcommand{\citeform}[1]{\emph{#1}}
  \fi
\fi
```

If the babel package is loaded, the `note` option does not work. So it is disabled here with a suitable warning.

```
\@ifpackageloaded{babel}
  {\ACS@notefalse\PackageWarning{achemso}%
    {babel package loaded - note option disabled}}
  {}
```

`\ACS@biberror` The function `\ACS@biberror` is defined here to provide an easy way of generating a warning if there is no name for a bibliography section. This will only happen with non-standard class files.

```
\newcommand*{\ACS@biberror}{\PackageError{achemso}%
  {No bibliography name command defined}
  {The document class you have used does not define
    \string\refname\MessageBreak or \string\bibname}}
```

`\refname` `\bibname` The `note` option renames the references section to "References and Notes". This applies for all standard document classes. The term "Bibliography" is not used in chemistry, the value of `\bibname` is redefined here in all cases where it exists.

```
\@ifundefined{refname}{%
  \@ifundefined{bibname}{%
    \ACS@biberror
  }{%
    \ifACS@note
      \renewcommand*{\bibname}{References and Notes}
    \else
      \renewcommand*{\bibname}{References}
    \fi
  }
}{%
  \ifACS@note
    \renewcommand*{\refname}{References and Notes}
  \fi
}
```

If the `number` option is set, the tocbibind package is used to number the bibliography.

```
\ifACS@sctnnmbr
  \RequirePackage[numbib]{tocbibind}
\fi
```

\bibliographystyle
\acs@bibstyle

Depending on the package option, the bibliography style will either be `achemso` or `achemsol`. The later is intended for listing the entire database. The `list` option of the package selects this, and for listing also generates boxed labels for each reference. The showkeys package provides this functionality. If natbib is asked for, then the appropriate style files are used in place of the standard ones.

```
\ifACS@mcite
  \RequirePackage{mciteplus}
\fi
\ifACS@iecr
  \ifACS@natbib
    \ifACS@mcite
      \newcommand*{\acs@bibstyle}{iecrnatM}%
    \else
      \newcommand*{\acs@bibstyle}{iecrnat}%
    \fi
  \else
    \ifACS@mcite
      \newcommand*{\acs@bibstyle}{iecrM}%
    \else
      \newcommand*{\acs@bibstyle}{iecr}%
    \fi
  \fi
\else
  \ifACS@list
    \ifACS@natbib
        \ifACS@mcite
          \newcommand*{\acs@bibstyle}{achemlntM}%
        \else
          \newcommand*{\acs@bibstyle}{achemlnt}%
        \fi
    \else
      \ifACS@mcite
        \newcommand*{\acs@bibstyle}{achemsolM}%
      \else
        \newcommand*{\acs@bibstyle}{achemsol}%
      \fi
    \fi
    \RequirePackage[notcite]{showkeys}
  \else
    \ifACS@natbib
        \ifACS@mcite
          \newcommand*{\acs@bibstyle}{achemnatM}%
        \else
          \newcommand*{\acs@bibstyle}{achemnat}%
        \fi
    \else
      \ifACS@mcite
        \newcommand*{\acs@bibstyle}{achemsoM}%
      \else
        \newcommand*{\acs@bibstyle}{achemso}%
      \fi
    \fi
  \fi
```

```
\fi
\expandafter\bibliographystyle\expandafter{\acs@bibstyle}
```

`\@biblabel` In order to re-format the bibliography labels, the easiest method is to redefine the `\@biblabel` macro from the LaTeX kernel.

```
\ifACS@iecr
  \renewcommand*{\@biblabel}[1]{(#1)}
\else
  \renewcommand*{\@biblabel}[1]{#1.}
\fi
```

`\ACS@bibwarning` `\acs@bibliographystyle` To ensure that additional `\bibliographystyle` commands in the source are killed off. The `\ACS@bibwarning` provides a clean method of generating the warning message.

```
\let\acs@bibliographystyle\bibliographystyle
\newcommand*{\ACS@bibwarning}{\PackageWarning{achemso}%
  {Additional bibliographystyle command ignored}}
\AtBeginDocument{
  \@ifpackageloaded{chapterbib}{\let\ACS@bibwarning\relax}{}}
\renewcommand*{\bibliographystyle}{%
  \expandafter\acs@bibliographystyle\expandafter{\acs@bibstyle}%
  \ACS@bibwarning\@gobble}
```

The package is complete.

```
⟨/package⟩
```

5 Change History

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.

7 References

1. *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.

2. http://pubs.acs.org/books/references.shtml.