

The `achemso` package — A BibTeX style 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 is a BibTeX style file to be used for bibliography database listings.

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.

This package consists of two BibTeX files (`achemso.bst` and `achemsol.bst`) 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 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 “American *Chemical Society*.”

*This file has version number v2.1, last revised 2007/02/15.

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

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

| Journal Title | CASSI Abbreviation |
|---|-------------------------------|
| <i>ACS Chemical Biology</i> | <i>ACS Chem. Biol.</i> |
| <i>Bioconjugate Chemistry</i> | <i>Bioconjugate Chem.</i> |
| <i>Biotechnology Progress</i> | <i>Biotechnol. Prog.</i> |
| <i>Chemical Research in Toxicology</i> | <i>Chem. Res. Toxicol.</i> |
| <i>Environmental Science and Technology</i> | <i>Environ. Sci. Technol.</i> |
| <i>Journal of Agricultural and Food Chemistry</i> | <i>J. Agric. Food Chem.</i> |

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

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 `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; the consensus of current practice in *Journal of the American Chemical Society* 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 only need the title of the book; the title of the subunit (given in `title`) is again ignored. This is the practice in *Journal of the American Chemical Society*: some of the other journals may take a different approach.

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 $\{\langle text \rangle\}$, and gives the output **Referenced in: text**. This command takes one argument (normally text) which is preceded by the text “**Referenced in: $\langle text \rangle$** ”. 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 writers 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.

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` package), and the package ensures that the bibliography will be named “References” in all standard document types.¹

The `achemso` package has four options: `note`, `list`, and `number`:

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.

¹This only works if the `babel` package is *not* loaded.

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 `achemso1`, 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.

4 The Package Code

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

`\ACSver` An identifying macro is provided, so that other packages can detect the version of `achemso` in use.

```
1 \*package
2 \def\ACSver{\texttt{achemso} v2.1 (2007/02/15)}
```

`\ACS@sctnnmbr` Four Boolean values are used to handle the options.

```
\ACS@lst 3 \newif \ifACS@sctnnmbr \ACS@sctnnmbrfalse
\ACS@note 4 \newif \ifACS@lst \ACS@lstfalse
\ACS@super 5 \newif \ifACS@note \ACS@notefalse
6 \newif \ifACS@super \ACS@supertrue
```

The options are processed.

```
7 \DeclareOption{note}{\global\ACS@notetrue}
8 \DeclareOption{number}{\global\ACS@sctnnmbrtrue}
9 \DeclareOption{list}{}
10 \DeclareOption{notsuper}{\global\ACS@superfalse}
11 \DeclareOption*{\OptionNotUsed}
12 \ProcessOptions
```

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.

```
13 \ifACS@super
14 \RequirePackage[super,nospace]{cite}
15 \else
16 \RequirePackage{cite}
17 \def\citeleft{()}
18 \def\citeright{)}
19 \def\citeform{\emph{#1}}
20 \fi
```

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

```
21 \ifpackageloaded{babel}
22 {\ACS@notefalse\PackageWarning{achemso}%
```

```

23     {babel package loaded - note option disabled}}
24     {\relax}

\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.
25 \def\ACS@biberror{\PackageError{achemso}%
26   {No bibliography name command defined}\@eha}

\refname The note option renames the references section to “References and Notes”. This
\bibname 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.
27 \ifx\refname\undefined
28   \ifx\bibname\undefined
29     \ACS@biberror
30   \else
31     \ifACS@note
32       \renewcommand*{\bibname}{References and Notes}
33     \else
34       \renewcommand*{\bibname}{References}
35     \fi
36   \fi
37 \else
38   \ifACS@note
39     \renewcommand*{\refname}{References and Notes}
40   \fi
41 \fi

If the number option is set, the tocbibind package is used to number the bibliog-
raphy.
42 \ifACS@sctnmbr
43   \RequirePackage[numbib]{tocbibind}
44 \fi

\bibliographystyle 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.
45 \ifACS@lst
46   \bibliographystyle{achemsol}
47   \RequirePackage[notcite]{showkeys}
48 \else
49   \bibliographystyle{achemso}
50 \fi

\@biblabel In order to re-format the bibliography labels, the easiest method is to redefine the
\@biblabel macro from the LaTeX kernel.
51 \def\@biblabel#1{#1.}

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

```

```

52 \def\ACS@bibwarning{\PackageWarning{achemso}%
53 {Additional bibliographystyle command ignored}}
54 \def\bibliographystyle{\ACS@bibwarning\@gobble}

```

The package is complete.

```
55 \end{package}
```

Change History

| | | | |
|-------------------------------------|---|-----------------------------------|---|
| v1.0 | | \bibliographystyle: Command | |
| General: Initial release of package | | ignored in document body | 6 |
| by Mats Dahlgren | 1 | Replaced custom code with | |
| v2.0 | | showkeys package | 6 |
| General: License changed to LPPL | 1 | v2.1 | |
| Re-write of package by Joseph | | General: BibTeX style improved to | |
| Wright | 1 | reflect 3rd edition of ACS Style | |
| Several improvements to BibTeX | | Guide | 1 |
| style files | 1 | Updated documentation to re- | |
| Switched to using tocbind to | | fect 3rd edition of ACS Style | |
| produce number bibliography . | 6 | Guide | 1 |
| \ACS@note: Boolean values made | | \ACS@super: New Boolean for cita- | |
| internal to package | 5 | tion control | 5 |

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>.

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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.

| | | |
|------------------------------------|------------------------------------|------------------------------|
| Symbols | \ACS@sctnnmbrtrue . . 8 | \citeleft 17 |
| \@biblabel <u>51</u> | \ACS@super <u>3</u> | \citeright 18 |
| | \ACS@superfalse . . . 10 | |
| A | \ACS@supertrue 6 | I |
| \ACS@biberror . . . <u>25</u> , 29 | \ACSver <u>1</u> | \ifACS@lst 4, 45 |
| \ACS@bibwarning . . . <u>52</u> | | \ifACS@note . . . 5, 31, 38 |
| \ACS@lst <u>3</u> | B | \ifACS@sctnnmbr . . 3, 42 |
| \ACS@lstfalse 4 | \bibliographystyle . | \ifACS@super 6, 13 |
| \ACS@note <u>3</u> | 4, <u>45</u> , <u>52</u> | |
| \ACS@notefalse . . . 5, 22 | \bibname <u>27</u> | R |
| \ACS@notetrue 7 | | \refin 4 |
| \ACS@sctnnmbr <u>3</u> | C | \refname <u>27</u> |
| \ACS@sctnnmbrfalse . . 3 | \citeform 19 | |