

# achemso— $\text{\LaTeX}$ and $\text{\BibTeX}$ support for American Chemical Society publications\*

Joseph Wright<sup>†</sup>

Released 2008/01/21

## Abstract

The `achemso` package provides a  $\text{\BibTeX}$  style in accordance with the requirements of the journals of the American Chemical Society, along with a supporting  $\text{\LaTeX}$  package file. Also provided are a number of  $\text{\BibTeX}$  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  $\text{\LaTeX}$  for the preparation of journal articles. Some journals, mainly in the physical chemistry area, do accept  $\text{\LaTeX}$  submissions. Given the clear advantages of  $\text{\LaTeX}$  over other methods, it would be nice to be able to use  $\text{\LaTeX}$  for preparing reports. Thus the need for  $\text{\BibTeX}$  styles for chemistry is real. The package `achemso` provides for a  $\text{\BibTeX}$  style and other support for articles and reports in the style of the American Chemical Society (ACS).

As describe in *The ACS Style Guide*,<sup>1</sup> almost all ACS publications use the same style for the formatting of references. The reproduction of this style is the aim of the  $\text{\BibTeX}$  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  $\text{\BibTeX}$  files along with a small  $\text{\LaTeX}$  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  $\text{\LaTeX}$  2.09 and  $\text{\BibTeX}$  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

---

\*This file describes version v2.2g, last revised 2008/01/21.

<sup>†</sup>E-mail: joseph.wright@morningstar2.co.uk

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 &amp; Design</i>	<i>Cryst. Growth Des.</i>
<i>Energy &amp; Fuels</i>	<i>Energy Fuels</i>
<i>Industrial &amp; 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 &amp; 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

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.”

### 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*,<sup>1</sup> on the ACS website,<sup>2</sup> 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  $\text{\LaTeX}$  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  $\text{\BibTeX}$  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 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,  $\text{\BibTeX}$  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 L<sup>A</sup>T<sub>E</sub>X 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.<sup>1</sup>

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.*<sup>3</sup>) 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`.

---

<sup>1</sup>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*.

## 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.

```
1 \*package
2 \NeedsTeXFormat{LaTeX2e}
3 \ProvidesPackage{achemso}
4   [2008/01/21 v2.2g LaTeX and BibTeX support for American
5     Chemical Society publications]
```

```
\ifACS@sctnnmbr Boolean values are used to handle the options.
\ifACS@list      6 \newif\ifACS@sctnnmbr\ACS@sctnnmbrfalse
\ifACS@note      7 \newif\ifACS@list\ACS@listfalse
\ifACS@super     8 \newif\ifACS@note\ACS@notefalse
\ifACS@natbib    9 \newif\ifACS@super\ACS@supertrue
\ifACS@mcite    10 \newif\ifACS@natbib\ACS@natbibfalse
\ifACS@iecr     11 \newif\ifACS@mcite\ACS@mcitelfalse
                12 \newif\ifACS@iecr\ACS@iecrfalse
```

The options are processed.

```
13 \DeclareOption{note}{\ExecuteOptions{notes}}
14 \DeclareOption{notes}{\ACS@notetrue}
15 \DeclareOption{number}{\ACS@sctnnmbrtrue}
16 \DeclareOption{super}{\ACS@supertrue}
17 \DeclareOption{list}{\ACS@listtrue}
18 \DeclareOption{notsuper}{\ACS@superfalse}
19 \DeclareOption{natbib}{\ACS@natbibtrue}
20 \DeclareOption{mcite}{\ACS@mcitetrue}
21 \DeclareOption{iecr}{\ACS@iecrtrue}
22 \DeclareOption*{\OptionNotUsed}
23 \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.

```
24 \ifACS@natbib
25   \ifACS@super
26     \RequirePackage[numbers,sort&compress,super]{natbib}
27   \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.
```

```
28   \RequirePackage[numbers,sort&compress,round]{natbib}
29   \newcommand*{\citenumfont}{\textit}
30   \fi
31 \else
32   \ifACS@super
```

```

33   \RequirePackage[nospace]{overcite}
34   \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.

```

35   \RequirePackage{cite}
36   \renewcommand{\citeleft}{({}
37   \renewcommand{\citeright}{)}
38   \renewcommand{\citeform}[1]{\emph{#1}}
39   \fi
40 \fi

```

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

```

41 \@ifpackageloaded{babel}
42   {\ACS@notefalse\PackageWarning{achemso}%
43     {babel package loaded - note option disabled}}
44   {}

```

`\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.

```

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

```

`\refname` 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.

`\bibname`

```

49 \@ifundefined{refname}{%
50   \@ifundefined{bibname}{%
51     \ACS@biberror
52   }{%
53     \ifACS@note
54       \renewcommand*{\bibname}{References and Notes}
55     \else
56       \renewcommand*{\bibname}{References}
57     \fi
58   }
59 }{%
60   \ifACS@note
61     \renewcommand*{\refname}{References and Notes}
62   \fi
63 }

```

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

```

64 \ifACS@sctnnmbr
65   \RequirePackage[numbib]{tocbibind}
66 \fi

```

`\bibliographystyle` Depending on the package option, the bibliography style will either be `achemso` or `achemso1`. 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.

```

67 \ifACS@mcite
68   \RequirePackage{mciteplus}
69 \fi
70 \ifACS@iecr
71   \ifACS@natbib
72     \ifACS@mcite
73       \bibliographystyle{iecrnatM}
74     \else
75       \bibliographystyle{iecrnat}
76     \fi
77   \else
78     \ifACS@mcite
79       \bibliographystyle{iecrM}
80     \else
81       \bibliographystyle{iecr}
82     \fi
83   \fi
84 \else
85   \ifACS@list
86     \ifACS@natbib
87       \ifACS@mcite
88         \bibliographystyle{achemlntM}
89       \else
90         \bibliographystyle{achemlnt}
91       \fi
92     \else
93       \ifACS@mcite
94         \bibliographystyle{achemsolM}
95       \else
96         \bibliographystyle{achemsol}
97       \fi
98     \fi
99     \RequirePackage[notcite]{showkeys}
100 \else
101   \ifACS@natbib
102     \ifACS@mcite
103       \bibliographystyle{achemnatM}
104     \else
105       \bibliographystyle{achemnat}
106     \fi
107   \else
108     \ifACS@mcite
109       \bibliographystyle{achemsoM}
110     \else
111       \bibliographystyle{achemso}
112     \fi
113   \fi
114 \fi
115 \fi

```

\@biblabel In order to re-format the bibliography labels, the easiest method is to redefine



the `\@biblabel` macro from the  $\text{\LaTeX}$  kernel.

```
116 \ifACS@iecr
117   \renewcommand*{\@biblabel}[1]{(#1)}
118 \else
119   \renewcommand*{\@biblabel}[1]{#1.}
120 \fi
```

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

```
121 \newcommand*{\ACS@bibwarning}{\PackageWarning{achemso}%
122   {Additional bibliographystyle command ignored}}
123 \renewcommand*{\bibliographystyle}{\ACS@bibwarning\@gobble}
```

The package is complete.

```
124 \end{package}
```

## 5 Change History

v1.0	General: Initial release of package by Mats Dahlgren . . . . .	1	title field included in output for incollection records . . .	1
v2.0	General: License changed to LPPL .	1	Bug fixes to natbib and list support . . . . .	1
	Re-write of package by Joseph Wright . . . . .	1	Fixed separation of editor names	1
	Several improvements to BibTeX style files . . . . .	1	<code>\ifACS@natbib</code> : New Boolean for natbib support . . . . .	6
	Switched to using tocbibind to produce number bibliography . . . .	7	v2.2b	
	<code>\bibliographystyle</code> : Command ignored in document body . . . . .	9	General: Bug fix to name formatting	1
	Replaced custom code with showkeys package . . . . .	7	v2.2c	
	<code>\ifACS@note</code> : Boolean values made internal to package . . . .	6	General: Use the overcite alias for cite as ACS have very old $\text{\LaTeX}$ system . . . . .	7
v2.1	General: cite package is loaded with different options depending on citation style requested . . . . .	6	v2.2d	
	BibTeX style improved to reflect 3rd edition of ACS Style Guide .	1	General: Added URL field to misc output . . . . .	1
	Updated documentation to reflect 3rd edition of ACS Style Guide .	1	Added notes option . . . . .	6
	<code>\ifACS@super</code> : New Boolean for citation control . . . . .	6	Package design improved . . . .	1
v2.2	General: Added natbib support . . .	1	v2.2e	
v2.2a	General: natbib support added . . . .	6	General: Added mciteplus support .	1
			Documentation improvements . .	1
			<code>\ACS@biberror</code> : Improved error message . . . . .	7
			<code>\ifACS@mcite</code> : New macro . . . .	6
			v2.2f	
			General: Combined mciteplus and natbib support . . . . .	1
			v2.2g	
			<code>\@biblabel</code> : Added <code>iecr</code> option to code . . . . .	8
			General: Support for <i>Industrial &amp; Engineering Chemistry Research</i> . . . .	1

<code>\bibliographystyle:</code>	Added	<code>iecr code</code>	..... 7
		<code>\ifACS@iecr: New macro</code>	..... 6

## 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.

Symbols			I
<code>\@biblabel</code> .....	<u>116</u>	<code>\ACS@notetrue</code> ....	14
		<code>\ACS@sctnnmbrfalse</code>	..... 6
<b>A</b>		<code>\ACS@sctnnmbrtrue</code>	15
<code>\ACS@biberror</code> ..	<u>45</u> , 51	<code>\ACS@superfalse</code> ..	18
<code>\ACS@bibwarning</code> .	<u>121</u>	<code>\ACS@supertrue</code> .	9, 16
<code>\ACS@iecrfalse</code> ...	12		
<code>\ACS@iecrtrue</code> ....	21		
<code>\ACS@listfalse</code> ....	7	<b>B</b>	
<code>\ACS@listtrue</code> ....	17	<code>\bibliographystyle</code>	..... <u>5</u> , <u>67</u> , <u>121</u>
<code>\ACS@mcitefalse</code> ..	11	<code>\bibname</code> .....	<u>48</u> , <u>49</u>
<code>\ACS@mcitetrue</code> ...	20		
<code>\ACS@natbibfalse</code> .	10	<b>C</b>	
<code>\ACS@natbibtrue</code> ..	19	<code>\citenumfont</code> .....	<u>28</u>
<code>\ACS@notefalse</code> .	8, <u>42</u>		
		<b>R</b>	
		<code>\refin</code> .....	<u>4</u>
		<code>\refname</code> .....	<u>48</u> , <u>49</u>

## 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>.