# 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.

#### Contents

#### 1 Introduction

Support for BIBT<sub>E</sub>X 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  $2_{\mathcal{E}}$  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.

<sup>\*</sup>This file describes version v3.12, last revised 2018/09/15.

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<sup>&</sup>lt;sup>1</sup>For example, when writing a thesis.

### 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
- geometry
- natbib
- setspace
- xkeyval

These are normally present in the current major T<sub>E</sub>X distributions, but are also available from The Comprehensive TeX Archive Network.

## 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.

Journal	Setting	Journal	Setting
Acc. Chem. Res.	achre4	Chem. Res. Toxicol.	crtoec
ACS Appl. Energy Mater.	aaemcq	Chem. Rev.	chreay
ACS Appl. Electron. Mater.	aaembp	Cryst. Growth Des.	cgdefu
ACS Appl. Mater. Interfaces	aamick	Energy Fuels	enfuem
ACS Appl. Nano Mater.	aanmf6	Environ. Sci. Technol.	esthag
ACS Appl. Polym. Mater.	aapmcd	Environ. Sci. Technol. Lett.	estlcu
ACS Biomater. Sci. Eng.	abseba	Ind. Eng. Chem. Res.	iecred
ACS Catal.	accacs	Inorg. Chem.	inoraj
ACS Central Sci.	acscii	J. Agric. Food Chem.	jafcau
ACS Chem. Biol.	acbcct	J. Chem. Ed.	jceda8
ACS Chem. Neurosci.	acncdm	J. Chem. Eng. Data	jceaax
ACS Combinatorial Sci.	acsccc	J. Chem. Inf. Model.	jcisd8
ACS Earth Space Chem.	aesccq	J. Chem. Theory Comput.	jctcce
ACS Energy Lett.	aelccp	J. Med. Chem.	${\tt jmcmar}$
ACS Infect. Dis.	ascefj	J. Nat. Prod.	jnprdf
ACS Macro Lett.	amlccd	J. Org. Chem.	joceah
ACS Med. Chem. Lett.	amclct	J. Phys. Chem. A	jpcafh
ACS Nano	ancac3	J. Phys. Chem. B	jpcbfk
ACS Omega	acsodf	J. Phys. Chem. C	jpccck
ACS Photon.	apchd5	J. Phys. Chem. Lett.	jpclcd
ACS Sensors	ascefj	J. Proteome Res.	jprobs
ACS Sustainable Chem. Eng.	ascecg	J. Am. Chem. Soc.	jacsat
ACS Synth. Biol.	asbcd6	Langmuir	langd5
Anal. Chem.	ancham	Macromolecules	mamobx
Biochemistry	bichaw	Mol. Pharm.	mpohbp
Bioconjugate Chem.	bcches	Nano Lett.	nalefd
Biomacromolecules	bomaf6	Org. Lett.	orlef7
Chem. Mater.	cmatex	Organometallics	orgnd7

Table 1: Values for journal option

#### 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 ??. 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, include the settings after the \documentclass line using \setkeys:

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

#### 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.² 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}
```

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}
```

<sup>&</sup>lt;sup>2</sup>This will usually be the university or company name.

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 \AbstractOff \AbstractOn 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 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.

\doi

The bibliography style prints any DOI values as the argument to the command \doi. The default definition will allow printing of special characters but does not create hyperlinks. A more sophisticated version of the command may be set up if hyperref is loaded, for example

```
\begin{tocentry}
  \newcommand{\doi}[1]{\href{http://dx.doi.org/#1}{\nolinkurl{#1}}}
\end{tocentry}
```

# 5 The package file

The achemso package is independent of the class 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

doi

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=true.

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.

#### 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  $\mathtt{BibT}_{EX}$ . 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.?

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.

# 6 The BibT<sub>E</sub>X 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 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.

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? some more text.
Some text ending a sentence.?
This is deactivated for other citation types.
```

```
Some text \citeyear{Coghill2006}.\\
Some text \citeauthor{Coghill2006}.\\
Some text \citenum{Coghill2006}.
Some text ?.
Some text ?.
```

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?, more text.?
                                       Some text \cite{Coghill2006},
                                       more text \cite{Coghill2006}.
```

#### **Implementation** 8

A lot of the work done by the package is also needed by the class. Loading the package and the class makes load-order awkward. Instead, the two parts are done in one place. Sandwiching the common code are two slices of dedicated material for the class and the package. Some of this is needed "early", before the common material, whilst the rest is "late".

#### Early class-only code

So that there is no confusion, the base class is loaded early.

```
_1 (*class)
2 \ProvidesClass{achemso}
   [2018/09/15 v3.12 Submission to ACS journals]
4 \LoadClass[12pt,letter]{article}
```

\acs@warning The code for a warning is created so that it works for the package too.

```
5 \newcommand*\acs@warning{\ClassWarning{achemso}}
6 (/class)
```

## Early package-only code

The package and the class should not both be loaded, as the two use the same internal macro names. On the other hand, if the class is not in use a reminder is printed to use it if possible.

```
_7 (*package)
8 \ProvidesPackage{achemso}
9 [2018/09/15 v3.12 Support for ACS journals]
10 \@ifclassloaded{achemso}{%
   \PackageInfo{achemso}{%
      You have already loaded the 'achemso' class:\MessageBreak
      loading the package will abort%
13
   }%
14
   \endinput
15
16 }{%
   \PackageInfo{achemso}{%
     When writing a submission to an ACS journal, please\MessageBreak
18
     use the achemso document class%
20 }%
21 }
```

The code for a warning is created so that it works for the class too. \acs@warning

```
22 \newcommand*\acs@warning{\PackageWarning{achemso}}
<sub>23</sub> ⟨/package⟩
```

#### Common code 8.3

\acs@ifundefined

A non-expandable test for defined macros: does not add to the hash table.

```
24 (*package | class)
25 \newcommand*\acs@ifundefined[1]{%
    \begingroup\expandafter\expandafter\expandafter\endgroup
26
    \expandafter\ifx\csname #1\endcsname\relax
27
      \expandafter\@firstoftwo
28
    \else
29
      \expandafter\@secondoftwo
30
    \fi
31
32 }
```

The first stage needed is to read the package options given. Although xkeyval was perhaps not the best choice, changing this now would be rather risky.

```
33 \RequirePackage{xkeyval}
```

41 \newif\ifacs@abbreviations

\acs@keyval@bool

A support macro for making Boolean options: the xkeyval version is only available in newer releases.

```
34 \newcommand*\acs@keyval@bool[2]{%
    \acs@ifundefined{acs@#1#2}{%
35
       \acs@warning{Unknown option '#2' for key #1}%
36
37
       \ensuremath{\mbox{\tt Qnameuse\{acs@\#1\#2\}\%}}
38
    }%
39
40 }
```

\ifacs@abbreviations \ifacs@articletitle \ifacs@biochem

\ifacs@chaptertitle \ifacs@keywords

\ifacs@super

These are all very trivial definitions: to avoid issues with older versions of xkeyval each definition is done directly.

```
42 \newif\ifacs@articletitle
   \ifacs@doi 43\newif\ifacs@biochem
\ifacs@email 44\newif\ifacs@doi
\ifacs@hyperref 45 \newif\ifacs@chaptertitle
                 46 \newif\ifacs@email
                  47 \newif\ifacs@hyperref
                   48 \newif\ifacs@keywords
                  49 \newif\ifacs@super
                   50 \define@key{acs}{abbreviations}[true]{%
                       \acs@keyval@bool{abbreviations}{#1}%
                   51
                  52 }
                   53 \define@key{acs}{articletitle}[true]{%
                       \acs@keyval@bool{articletitle}{#1}%
                   54
                  55 }
                   56 \define@key{acs}{biochem}[true]{%
                       \acs@keyval@bool{biochem}{#1}%
                  58 }
                   59 \define@key{acs}{doi}[true]{%
                   60 \acs@keyval@bool{doi}{#1}%
```

```
61 }
                          62 \define@key{acs}{chaptertitle}[true]{%
                              \acs@keyval@bool{chaptertitle}{#1}%
                          63
                          64 }
                          65 \define@key{acs}{email}[true]{%
                              \acs@keyval@bool{email}{#1}%
                          66
                          67 }
                          68 \define@key{acs}{hyperref}[true]{%
                              \acs@keyval@bool{hyperref}{#1}%
                          70 }
                          71 \define@key{acs}{keywords}[true]{%
                              \acs@keyval@bool{keywords}{#1}%
                          <sub>73</sub> }
                          _{74} \ensuremath{\mbox{define@key{acs}{super}[true]{\%}}
                              \acs@keyval@bool{super}{#1}%
                          75
                          76 }
                          77 \define@key{acs}{usetitle}[true]{%
                              \acs@keyval@bool{articletitle}{#1}%
                          79 }
          \acs@journal
                         Trivial again: done without using xkeyval for the same reasons as before.
           \acs@layout
                          80 \newcommand*\acs@journal{jacsat}
                         81 \newcommand*\acs@layout{traditional}
       \acs@manuscript
                         82 \newcommand*\acs@manuscript{article}
       \acs@maxauthors
                          83 \mbox{newcommand*}\acs@maxauthors{15}
                          84 \define@key{acs}{journal}{%
                              \def\acs@journal{#1}%
                          85
                          86 }
                          87 \define@key{acs}{layout}{%
                          88
                              \def\acs@layout{#1}%
                          89 }
                          90 \define@key{acs}{manuscript}{%
                              \def\acs@manuscript{#1}%
                          92 }
                          93 \define@key{acs}{maxauthors}{%
                              \def\acs@maxauthors{#1}%
                          95 }
                         The setup for the etalmode option is quite simple: just look for the appropriate
  \ifacs@etal@truncate
   \acs@etal@firstonly
                         macros.
    \acs@etal@truncate
                          96 \newif\ifacs@etal@truncate
                          97 \define@key{acs}{etalmode}{%
                              \acs@ifundefined{acs@etal@#1}{%
                          98
                                \acs@warning{%
                          99
                                  Unknown value '#1' for\MessageBreak etalmode option%
                         100
                                }%
                         101
                              }{%
                         102
                                \@nameuse{acs@etal@#1}%
                         103
                         104
                         105 }
                         106 \newcommand*\acs@etal@firstonly{\acs@etal@truncatefalse}
                         107 \newcommand*\acs@etal@truncate{\acs@etal@truncatetrue}
                         The biochemistry option is an alias for biochem. The biblabel option is a
\acs@activate@biblabel
```

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choice, which is implemented using a csname search. The group here prevents

hash table pollution, whilst the xkeyval method is avoided as it is more complex than it is worth!

```
108 \define@key{acs}{biochemistry}{%
                           \setkeys{acs}{biochem = #1}%
                      110}
                      111 \define@key{acs}{biblabel}{%
                           \acs@ifundefined{acs@biblabel@#1}{%
                      112
                             \acs@warning{%
                      113
                               Unknown value '#1' for\MessageBreak biblabel option%
                      114
                      115
                           }{%
                      116
                      117
                             \acs@activate@biblabel{\@nameuse{acs@biblabel@#1}}%
                      118
                           }%
                      119 }
                      120 \newcommand*\acs@activate@biblabel{}
                      121 (*class)
                      122 \let\acs@activate@biblabel\AtEndOfClass
                      123 \AtEndOfClass{\let\acs@activate@biblabel\@firstofone}
                      124 (/class)
                      125 (*package)
                      126 \let\acs@activate@biblabel\AtEndOfPackage
                      127 \AtEndOfPackage{\let\acs@activate@biblabel\@firstofone}
                      128 (/package)
                      The macros to implement the idea above for biblabels.
                      129 \newcommand*\acs@biblabel@brackets{\def\bibnumfmt##1{(##1)}}
\acs@biblabel@period 130 \newcommand*\acs@biblabel@fullstop{\def\bibnumfmt##1{##1.}}
 \acs@biblabel@plain 131\newcommand*\acs@biblabel@period{\def\bibnumfmt##1{##1.}}
                      132 \newcommand*\acs@biblabel@plain{\def\bibnumfmt##1{##1}}
                      Set up some defaults.
                      133 \setkeys{acs}{
                      134 email = true,
                          super = true
                      135
                       Loading some other packages depends on the options chosen, so they are pro-
                       cessed now.
                      137 \ProcessOptionsX*<acs>
                      For text comparisons.
                      138 \newcommand*\acs@manuscript@communication{communication}
                      139 \newcommand*\acs@manuscript@letter{letter}
                      140 \newcommand*\acs@manuscript@note{note}
                      142 \newcommand*\acs@manuscript@suppinfo{suppinfo}
```

\acs@manuscript@communication \acs@manuscript@letter \acs@manuscript@note \acs@manuscript@review

\acs@biblabel@brackets \acs@biblabel@fullstop

```
\acs@manuscript@suppinfo 141 \newcommand*\acs@manuscript@review{review}
```

\thebibnote \bibnote \bibnotetext

\printbibnotes

\acs@niib@create To avoid needing to load the notes2bib package, especially as the plan is to move bibnote that package to LATEX3 internal syntax, achemso provides a minimal version here. The first step is to create macros which will need a guard against notes2bib already having been loaded. To allow the package and class to behave differently \bibnotemark these are actually applied later.

143 \newcommand\*\acs@niib@create{%

```
2009/04/20 v1.6a Integrating notes into the bibliography (achemso
                         145
                                version)
                         146
                              }%
                         147
                              \@ifundefined{c@bibnote}{\newcounter{bibnote}}{}
                         148
                              \def\thebibnote{%
                         149
                                Note-\the\value{bibnote}%
                         150
                         151
                              \DeclareRobustCommand*{\bibnote}[1][\thebibnote]{%
                         152
                                \stepcounter{bibnote}%
                         153
                                \def\acs@niib@after@text{\cite{##1}}%
                         154
                                \acs@niib@text{##1}%
                         155
                         156
                              \DeclareRobustCommand*{\bibnotemark}[1][\thebibnote]{%
                         157
                                \stepcounter{bibnote}%
                         158
                                \cite{##1}%
                         159
                         160
                              \DeclareRobustCommand*{\bibnotetext}[1][\thebibnote]{%
                                \let\acs@niib@after@text\relax
                         162
                                \acs@niib@text{##1}%
                         163
                              }%
                         164
                              \newcommand*\printbibnotes{%
                         165
                                \ifnum\the\value{bibnote}>\z@\relax
                         166
                                   \nocite{achemso-control}%
                         167
                                   \acs@bibliography{acs-\jobname}%
                         168
                         169
                                \fi
                             }%
                         170
                         171 }
  \acs@niib@after@text After the text.
                         172 \newcommand*\acs@niib@after@text{}
        \acs@niib@text
                         The \acs@niib@text macro is the outer part of the writing system. It does not
                         absorb the text of note, as without \varepsilon-TEX this is bad news. The same file is used
                         for notes and the control entry for the bibliography style.
                         173 \newcommand*\acs@niib@text{%
                              \@bsphack
                         174
                              \if@filesw
                         175
                                \expandafter\acs@niib@write
                         176
                         177
                                \expandafter\acs@niib@no@write
                         178
                              \fi
                         179
                         180 }
                         Writing verbatim without \varepsilon-T<sub>E</sub>X.
       \acs@niib@write
 \acs@niib@write@aux@i
                         181 \newcommand*\acs@niib@write[1]{%
\acs@niib@write@aux@ii 182
                             \begingroup
                         183
                                \let\do\@makeother
                         184
                                \dospecials
                                \catcode'\{ 1\relax
                         185
                         186
                                \catcode'\} 2\relax
                                \acs@niib@write@aux@i{#1}%
                         187
                         188 }
                         189 \newcommand*\acs@niib@write@aux@i[1]{%
```

\@namedef{ver@notes2bib.sty}{%

144

```
\long\def\@tempa##1{%}
                     190
                              \def\@tempa{##1}%
                     191
                              \@onelevel@sanitize\@tempa
                     192
                            \expandafter\endgroup
                     193
                            \expandafter\def\expandafter\0tempa\expandafter{\0tempa}%
                     194
                            \acs@niib@write@aux@ii{#1}%
                     195
                     196
                          \catcode'\^^M 10\relax
                     197
                     198
                          \@tempa
                     199 }
                     200 \newcommand*\acs@niib@write@aux@ii[1]{%
                          \immediate\write\acs@bib@file{%
                     201
                            @Misc\string{#1,^^J%
                     202
                            \space\space note = \string{\@tempa\string}, ^^J%
                     203
                            \string}^^J%
                     204
                          }%
                     205
                          \@esphack
                     206
                          \acs@niib@after@text
                     207
                     208 }
                     If no files are to be written, a bit of tidying up.
\acs@niib@no@write
                     209 \newcommand\acs@niib@no@write[2]{%
                          \@esphack
                     210
                          \acs@niib@after@text
                     211
                     212 }
                     The functionality of notes2bib is combined with the standard \cite macro, to
\nmv@natbib@detect
                     give automatic note-like data in the bibliography.
 \acs@nmv@activate
     \acs@autonote
                    213 \AtBeginDocument{
                          \def\nmv@natbib@detect{%
                     214
                            \ifNAT@super
                     215
                              \expandafter\acs@nmv@activate
                     216
                            \else
                     217
                              \expandafter\acs@autonote
                     218
                            \fi
                     219
                     220
                     221 }
                     222 \newcommand*\acs@nmv@activate{%
                          \let\nmv@citex@nat\@citex
                     223
                          \let\@citex\nmv@citex
                          \let\nmv@cite\cite
                     225
                          \renewcommand*{\cite}[2][]{%
                     226
                            \nmv@ifmtarg{##1}{%
                     227
                              \nmv@citetrue
                     228
                              \nmv@cite{##2}%
                     229
                            }{%
                     230
                              \nocite{##2}%
                     231
                              \bibnote{Ref.~\citenum{##2}, ##1}%
                     232
                            }%
                     233
                         }%
                     234
                     235 }
                     236 \newcommand*\acs@autonote{%
                          \let\nmv@cite\cite
                          \renewcommand*{\cite}[2][]{%
```

```
239 \nmv@ifmtarg{##1}{%
240 \nmv@cite{##2}%
241 }{%
242 \nocite{##2}%
243 \bibnote{Ref.~\citenum{##2}, ##1}%
244 }%
245 }%
246}
```

\acs@bib@file \acs@bib@message \acs@bib@name Some information or creating the control file for BIBT<sub>E</sub>X is set up.

```
247 \newwrite\acs@bib@file
248 \newcommand*\acs@bib@message{%
249 This is an auxiliary file used by the 'achemso' bundle.^^J%
250 This file may safely be deleted. It will be recreated as required.^^J
251 }
252 \newcommand*\acs@bib@name{acs-\jobname.bib}
```

\acs@bib@write \acs@bib@write@aux

The control information for BibTeX needs to be written to a special file. The main writing macro is quite simple. Actually writing the information is left to the code for \bibliography, so that this only happens if needed.

```
253 \newcommand*\acs@bib@write{%
    \if@filesw
254
       \expandafter\acs@bib@write@aux
255
     \fi
256
257 }
258 \AtBeginDocument{\acs@bib@write}
259 \newcommand*\acs@bib@write@aux{%
     \immediate\openout\acs@bib@file\acs@bib@name\relax
261
     \immediate\write\acs@bib@file{\acs@bib@message}%
     \edef\@tempa##1##2{%
262
       \space\space##1\space = "##2",^^J%
263
    ጉ%
264
     \immediate\write\acs@bib@file{%
265
       @Control\string{%
266
         achemso-control,^^J%
267
         \@tempa{ctrl-article-title\space}{%
268
           \ifacs@articletitle yes\else no\fi
269
         }%
270
         \@tempa{ctrl-chapter-title\space}{%
271
           \ifacs@chaptertitle yes\else no\fi
272
273
         \@tempa{ctrl-doi\space\space\space\space\space\space
274
           \space\space\space\space\{%
275
           \ifacs@doi yes\else no\fi
276
277
         \@tempa{ctrl-etal-number\space\space\space}{\acs@maxauthors}%
278
         \@tempa{ctrl-etal-firstonly}{%
279
280
           \ifacs@etal@truncate no\else yes\fi
         }%
281
       \string}^^J%
282
283
     \immediate\write\@auxout{%
284
      \string\citation\string{achemso-control\string}%
285
286
    }%
```

```
287 \AtEndDocument{%
288 \immediate\closeout\acs@bib@file\relax
289 }%
290 }

\acs@bibliography The \bibliography macro is now patched so that everything works correctly.
\bibliography
291 \AtBeginDocument{%
292 \let\acs@bibliography\bibliography
293 \def\bibliography#1{%
294 \acs@bibliography{acs-\jobname,#1}%
295 }%
```

\latin The journal ACS Nano formats Latin phrases differently from every other ACS journal: we provide a \latin command to cover this.

```
297 \AtBeginDocument{
298 \providecommand{\latin}[1]{#1}
299 }
300 \( / \package \| \class \)
```

#### 8.4 Late class-only code

296 }

Most of the power of the class is now created. First, a few options are reset so that any given by the user are effectively ignored.

```
301 (*class)
302 \setkeys{acs}{
303 abbreviations = false,
304 articletitle = true,
305 biblabel = brackets,
306 biochem = false,
307 doi = false,
308 etalmode = firstonly,
309 keywords = false,
310 maxauthors = 15,
311 super = true
312}
```

When using the class, notes2bib is always emulated. Other standard support packages can now be loaded.

```
313 \acs@niib@create
314 \RequirePackage[margin=2.54cm] {geometry}
315 \RequirePackage{
316 caption,
317 float,
318 graphicx,
319 setspace,
320 url
321 }
322 \ifacs@hyperref
323 \expandafter\RequirePackage
324 \else
325 \expandafter\@gobble
326 \fi
```

```
327 {hyperref}
                       328 \AtBeginDocument{\doublespacing}
               \title For the meta-data, the REVTEX bundle provides a good model for the commands
              \@title to give the author. \gdef is used here to avoid any odd grouping issues.
     \acs@title@short
                       329 \renewcommand*{\title}[2][]{%
                           \gdef\acs@title@short{#1}%
                       331
                            \gdef\@title{#2}%
                            \ifx\acs@title@short\@empty
                             \global\let\acs@title@short\@title
                       334
                            \fi
                       335 }
                       336 \@onlypreamble\title
      \acs@author@cnt achemso tracks the number authors, affiliations and alternative affiliations.
       \acs@affil@cnt
                       337 \newcount\acs@author@cnt
   \acs@affil@alt@cnt 338 \newcount\acs@affil@cnt
                       339 \newcount\acs@affil@alt@cnt
    \acs@footnote@cnt Two counts for getting affiliation footnotes correct.
\acs@affil@marker@cnt
                       340 \newcount\acs@footnote@cnt
                       341 \newcount\acs@affil@marker@cnt
              \author The author macro stores the current author details and sets the affiliation of the
                       author to the current one. Everything is \global so that there is no possibility
                       of begin trapped inside a group. The affiliation counter is always one behind,
                       and so it is locally incremented to keep the logic of the code clear elsewhere.
                       342 \left\ \frac{1}{\%} \right
                            \global\advance\acs@author@cnt\@ne\relax
                       343
                            \expandafter\gdef\csname @author@\@roman\acs@author@cnt\endcsname{#1}%
                       344
                            \begingroup
                       345
                              \advance\acs@affil@cnt\@ne
                       346
                              \expandafter\xdef\csname @author@affil@\@roman
                       347
                                \acs@author@cnt\endcsname
                       348
                                {\the\acs@affil@cnt}%
                            \endgroup
                       350
                       351 }
                       352 \@onlypreamble\author
                 \and Neither \and nor \thanks are used by the document class.
              354 \acs@warning{%
                              \string\and\space not used by the achemso class: please see
                              the\MessageBreak package documentation for details%
                       356
                           }%
                       357
                       358 }
                       359 \def\thanks{%
                           \acs@warning{%
                              \string\thanks\space not used by the achemso class: please see
                              the\MessageBreak the package documentation for details%
                       363 }%
                       364 }
```

\affiliation As with \author, everything is \global just in case. The system insists that affiliations come after authors. Before anything is committed, a check is made that the affiliation has not already been seen.

365 \newcommand\*\affiliation[2][\relax]{%

```
\ifnum\acs@author@cnt>\z@\relax
                              \acs@affil@ifdup{#2}{%
                       367
                                \acs@affil@swap{#2}%
                       368
                              }{%
                       369
                                \global\advance\acs@affil@cnt\@ne\relax
                       370
                                \expandafter\gdef\csname @address@\@roman\acs@affil@cnt\endcsname
                       371
                                  {#2}%
                       372
                                \int x = 1 = x 
                       373
                                  \expandafter\gdef\csname @affil@\@roman\acs@affil@cnt\endcsname
                       374
                       375
                       376
                                  \expandafter\gdef\csname @affil@\@roman\acs@affil@cnt\endcsname
                       377
                       378
                                    {#1}%
                                \fi
                       379
                              }%
                       380
                            \else
                       381
                              \acs@warning{Affiliation with no author}%
                       382
                       383
                            \fi
                       385 \@onlypreamble\affiliation
    \acs@affil@ifdup A short test for two addresses being identical.
\acs@affil@ifdup@aux
                      386 \newcommand*\acs@affil@ifdup[1]{%
                           \begingroup
                       387
                              \def\@tempa{#1}%
                       388
                              \@tempswafalse
                       389
                              \@tempcnta\z@\relax
                       390
                              \acs@affil@ifdup@aux
                       391
                              \if@tempswa
                       392
                                \aftergroup\@firstoftwo
                       393
                              \else
                       394
                                \aftergroup\@secondoftwo
                       395
                              \fi
                       396
                            \endgroup
                       397
                       398 }
                       399 \newcommand*\acs@affil@ifdup@aux{%
                            \advance\@tempcnta\@ne\relax
                       400
                            \expandafter\expandafter\expandafter\def\expandafter\expandafter
                       401
                              \expandafter\@tempb\expandafter\expandafter\expandafter
                       402
                              {\csname @address@\@roman\@tempcnta\endcsname}%
                       403
                            \ifx\@tempa\@tempb
                       404
                              \expandafter\@tempswatrue
                       405
                            \else
                       406
                              \ifnum\@tempcnta<\acs@affil@cnt\relax
                       407
                                \expandafter\expandafter\expandafter\acs@affil@ifdup@aux
                       408
                              \fi
                       409
                           \fi
                       410
```

\acs@affil@swap \acs@affil@swap@aux 411 }

If the affiliation has already been given, then all of the authors need to be

checked to make sure that the correct affiliation is used. First, the loop from above is used to find the correct number for the duplicate.

```
412 \newcommand*\acs@affil@swap[1]{%
    \begingroup
413
       \def\@tempa{#1}%
414
       \@tempcnta\z@\relax
415
       \@tempcntb\z@\relax
416
       \acs@affil@ifdup@aux
417
418
       \advance\acs@affil@cnt\@ne\relax
419
       \acs@affil@swap@aux
420
     \endgroup
421 }
422 \newcommand*\acs@affil@swap@aux{%
     \advance\@tempcntb\@ne\relax
     \expandafter\ifnum\csname @author@affil@\@roman\@tempcntb\endcsname
424
       = \acs@affil@cnt\relax
425
       \expandafter\xdef\csname @author@affil@\@roman\@tempcntb\endcsname{%
426
         \the\@tempcnta
427
       }%
428
    \fi
429
     \ifnum\@tempcntb<\acs@author@cnt\relax
430
       \expandafter\acs@affil@swap@aux
431
432
     \fi
433 }
```

\alsoaffiliation \acs@alsoaffil@find

To allow complex affiliations , two commands are needed. The first deals with affiliations that are in some way shared by several authors. This is tracked on a per author basis.

```
434 \newcommand*\alsoaffiliation[2][\relax]{%
    \ifnum\acs@author@cnt>\z@\relax
       \acs@affil@ifdup{#2}{%
436
         \acs@alsoaffil@find{#2}%
437
       }{%
438
         \global\advance\acs@affil@cnt\@ne\relax
439
         \@tempcnta\acs@affil@cnt\relax
440
         \expandafter\gdef\csname @address@\@roman\acs@affil@cnt\endcsname
441
442
         \int x^{relax#1}
443
           \expandafter\gdef\csname @affil@\@roman\acs@affil@cnt\endcsname
444
             {#2}%
445
         \else
446
           \expandafter\gdef\csname @affil@\@roman\acs@affil@cnt\endcsname
447
             {#1}%
448
         \fi
449
450
       \@ifundefined{@author@alsoaffil@\@roman\acs@author@cnt}{%
451
         \expandafter\xdef\csname @author@alsoaffil@\@roman\acs@author@cnt
452
           \endcsname{\the\@tempcnta}%
453
454
         \expandafter\xdef\csname @author@alsoaffil@\@roman\acs@author@cnt
455
           \endcsname{%
456
           \csname @author@alsoaffil@\@roman\acs@author@cnt\endcsname
457
           ,\the\@tempcnta
458
         }%
459
```

```
}%
460
     \else
461
       \acs@warning{Affiliation with no author}%
462
463
464 }
465 \newcommand*\acs@alsoaffil@find[1]{%
     \begingroup
466
       \def\@tempa{#1}%
467
       \@tempcnta\z@\relax
468
       \@tempcntb\z@\relax
469
       \acs@affil@ifdup@aux
470
     \expandafter\endgroup
     \expandafter\@tempcnta\the\@tempcnta\relax
472
473 }
```

\altaffiliation

For the alternative affiliation, a second count is kept, and the affiliation is "attached" to the author. The way these are stored means that the appropriate affiliation number can be recovered later, and so printed correctly when things get complex.

```
474 \newcommand*\altaffiliation[1]{%
     \ifnum\acs@author@cnt>\z@\relax
475
476
       \begingroup
         \acs@altaffil@ifdup{#1}{%
477
           \expandafter\xdef\csname @author@altaffil@\@roman\acs@author@cnt
478
             \endcsname{\the\@tempcnta}%
479
480
         }{%
           \global\advance\acs@affil@alt@cnt\@ne\relax
481
           \expandafter\gdef\csname @altaffil@\@roman\acs@affil@alt@cnt
482
             \endcsname{#1}%
483
           \expandafter\xdef\csname @author@altaffil@\@roman\acs@author@cnt
484
             \endcsname{\the\acs@affil@alt@cnt}%
485
         }%
486
487
       \endgroup
     \else
488
       \acs@warning{Affiliation with no author}%
489
     \fi
490
491 }
492 \@onlypreamble\altaffiliation
```

\acs@altaffil@ifdup \acs@altaffil@ifdup@aux This is very similar to the same routine for normal affiliations but with the appropriate name changes.

```
493 \newcommand*\acs@altaffil@ifdup[1]{%
    \def\@tempa{#1}%
494
     \@tempswafalse
495
     \@tempcnta\z@\relax
496
     \ifnum\acs@affil@alt@cnt>\z@\relax
497
       \expandafter\acs@altaffil@ifdup@aux
498
    \fi
499
     \if@tempswa
500
       \expandafter\@firstoftwo
501
    \else
502
       \expandafter\@secondoftwo
503
    \fi
504
505 }
```

```
506 \newcommand*\acs@altaffil@ifdup@aux{%
                     \advance\@tempcnta\@ne\relax
                     \expandafter\expandafter\expandafter\expandafter\expandafter
                 508
                        \expandafter\@tempb\expandafter\expandafter\expandafter
                 509
                        {\csname @altaffil@\@roman\@tempcnta\endcsname}%
                 510
                     \ifx\@tempa\@tempb
                 511
                        \expandafter\@tempswatrue
                 512
                      \else
                 513
                        \ifnum\@tempcnta<\acs@affil@alt@cnt\relax
                          \expandafter\expandafter\expandafter\acs@altaffil@ifdup@aux
                        \fi
                 516
                     \fi
                 517
                 518}
         \email E-mail addresses are attached to authors as well.
                 519 \newcommand*\email[1]{%
                     \ifnum\acs@author@cnt>\z@\relax
                        \expandafter\gdef\csname @email@\@roman\acs@author@cnt\endcsname
                 521
                 522
                      \else
                 523
                        \acs@warning{E-mail with no author}%
                 524
                      \fi
                 525
                 527 \@onlypreamble\email
           \fax Fax and phone numbers are similar.
         \phone _{528} \newcommand*\fax[1]{%
                     \ifnum\acs@author@cnt>\z@\relax
                 529
                        \expandafter\gdef\csname @fax@\@roman\acs@author@cnt\endcsname
                 530
                          {#1}%
                 531
                 532
                        \acs@warning{Fax number with no author}%
                 533
                     \fi
                 534
                 535 }
                 536 \@onlypreamble\fax
                 537 \newcommand*\phone[1]{%
                     \ifnum\acs@author@cnt>\z@\relax
                 538
                        \expandafter\gdef\csname @phone@\@roman\acs@author@cnt\endcsname
                 539
                 540
                 541
                        \acs@warning{Phone number with no author}%
                 542
                     \fi
                 543
                 544 }
                 545 \@onlypreamble\phone
\abbreviations Some journals use these.
\@abbreviations
                546 \newcommand*\abbreviations[1]{%
      \keywords 547
                      \gdef\@abbreviations{#1}%
     \@keywords 548}
                 549 \newcommand*\@abbreviations{}
                 550 \@onlypreamble\abbreviations
                 551 \newcommand*\keywords[1]{%
                 552 \gdef\@keywords{#1}%
                 553 }
```

```
554 \newcommand*\@keywords{}
                                                                                              555 \@onlypreamble\keywords
\acs@abbreviations@print
                                                                                              For printing the key simple meta-data.
                  \acs@keywords@print
                                                                                              556 \newcommand*\acs@abbreviations@print{%
       \acs@title@short@print
                                                                                                              \ifx\@abbreviations\@empty\else
                                                                                                                       \section*{Abbreviations}
                                                                                              558
                                                                                                                       \@abbreviations
                                                                                              559
                                                                                                                       \par
                                                                                              560
                                                                                              561
                                                                                                              \fi
                                                                                              562 }
                                                                                              563 \newcommand*\acs@keywords@print{%
                                                                                                               \ifx\@keywords\@empty\else
                                                                                                                       \section*{Keywords}
                                                                                              565
                                                                                                                       \@keywords
                                                                                                                       \par
                                                                                              568
                                                                                                            \fi
                                                                                              569 }
                                                                                              570 \newcommand*\acs@title@short@print{%
                                                                                                              \section*{Running header}
                                                                                                               \acs@title@short
                                                                                                               \par
                                                                                              573
                                                                                              574 }
                                                                                              Lengths for \@maketitle.
              \acs@space@pre@title
          \acs@space@post@title
                                                                                              575 \newlength\acs@space@pre@title
       \acs@space@post@author
                                                                                              576 \setlength\acs@space@pre@title{2em}
                                                                                              577 \newlength\acs@space@post@title
   \acs@space@post@address
                                                                                             578 \setlength\acs@space@post@title{1.5em}
          \acs@space@post@email
             \verb|\acs@maketitle@width | 579 \\ \verb|\newlength| acs@space@post@author | 1999 \\ \verb|\acs@maketitle@width | 1999 \\ \verb|\acs@maketitle
                                                                                              580 \setlength\acs@space@post@author{1em}
                                                                                              581 \newlength\acs@space@post@address
                                                                                              582 \setlength\acs@space@post@address{1em}
                                                                                              583 \newlength\acs@space@post@email
                                                                                              584\setlength\acs@space@post@email{1.5em}
                                                                                              585 \newlength\acs@maketitle@width
                                                                                              586 \setlength\acs@maketitle@width{\textwidth}
                                                  \affilsize Some simple size commands.
                                                \verb|\authorsize| _{587} \verb|\newcommand*| affilsize{\normalsize}|
                                                  \verb|\emailsize| 588 \verb|\emailsize| {\large}|
                                                  \titlesize 589 \newcommand*\emailsize{\normalsize}
                                                                                              590 \newcommand*\titlesize{\LARGE}
                                               \authorfont Font settings for \@maketitle.
                                               \verb|\authorfont| 591 \verb|\newcommand*\affilfont{$\o$ itshape}|
                                                  \label{lem:command*} $$\operatorname{lont}_{592} \end*\authorfont{\sffamily}$
                                                  \titlefont 593 \newcommand*\emailfont{}
                                                                                              _{594} \mbox{ } \mb
                                                              \ps@acs A shortcut to make page styles.
                                                                                              595 \newcommand*{\ps@acs}{}
                                                                                              596 \let\ps@acs\ps@plain
```

\@maketitle \@maketitle@hook

With the changes outlined above in place, a new \@maketitle macro is needed. This is partially a copy of the existing, but rather heavily modified.

```
597 \def\@maketitle{%
     \pagestyle{acs}%
     \ifnum\acs@author@cnt<\z@\relax
599
       \acs@warning{No authors defined: At least one author is required}%
600
     \fi
601
     \newpage
602
     \null
603
     \vspace*{\acs@space@pre@title}%
604
     \begin{center}
605
       \begin{minipage}{\acs@maketitle@width}
607
         \begin{center}
           {%
608
             \titlefont
609
             \titlesize
610
             \let\@fnsymbol\acs@author@fnsymbol
611
             \let\footnote\acs@title@footnote
612
             \acs@maketitle@suppinfo \@title
613
             \acs@title@footnote@check
614
              \global\acs@footnote@cnt\c@footnote
615
              \@maketitle@title@hook
616
617
              \par
           }%
618
           \vspace*{\acs@space@post@title}%
619
620
           {%
              \authorsize
621
              \authorfont
622
              \frenchspacing
623
              \acs@author@list
624
              \par
625
           }%
626
           \vspace*{\acs@space@post@author}%
627
628
           {%
              \affilsize
629
              \affilfont
630
              \acs@address@list
631
              \par
632
633
           \vspace*{\acs@space@post@address}%
634
635
              \emailsize
636
             \emailfont
637
             \ifacs@email
638
                \expandafter\acs@contact@details
639
              \fi
640
           }%
641
           \vspace*{\acs@space@post@email}%
642
         \end{center}
643
       \end{minipage}
644
     \end{center}%
645
646 }
647 \newcommand*\@maketitle@title@hook{}
```

```
This is spun out so that it can be avoided if necessary: this is done on the sly.
 \acs@maketitle@suppinfo
                           648 \newcommand*\acs@maketitle@suppinfo{%
                               \ifx\acs@manuscript\acs@manuscript@suppinfo
                                 Supporting Information:\\
                           650
                               \fi
                           651
                           652 }
      \acs@title@footnote Footnotes need to be created so that they appear correctly.
\acs@title@footnote@check
                          653 \newcommand*\acs@title@footnote[1]{%
                               \footnotemark
                           654
                                \g@addto@macro\@thanks{\footnotetext{#1}}%
                           655
                           656 }
                           657 \newcommand\acs@title@footnote@check{%
                           658
                               \ifx\@thanks\@empty
                           659
                               \else
                           660
                                 \begingroup
                                   \toks@=\expandafter{\@thanks}%
                           661
                                    \xdef\@thanks{%
                           662
                                      \begingroup
                           663
                                        664
                                        \the\toks@
                           665
                           666
                                      \endgroup
                                   }%
                           667
                           668
                                  \endgroup
                           669
                               \fi
                           670 }
    \acs@contact@details A general contact details macro.
                           671 \newcommand*\acs@contact@details{%
                           672 { \sffamily E-mail: \acs@email@list }%
                               \acs@number@list
                          673
                           674 }
                 \@thanks The \@thanks macro is used as a hook to generate the footnotes if needed.
                           675 \let\@thanks\@empty
        \acs@author@list
                          Printing the author list needs to do several things. The appropriate separators
                           between authors are created and the author names themselves are printed.
                           676 \newcommand*\acs@author@list{%
                           677
                               \@tempcnta\z@\relax
                               \ifnum\acs@author@cnt=\z@\relax\else
                           678
                                  \expandafter\acs@author@list@main
                           679
                           68o
                               \fi
                           681 }
                           The main control macro for producing the author list iterates over each author
   \acs@author@footnotes
                           on the list. The result is stored as \acs@author@listing.
   \acs@author@list@main
                           682 \newcommand*\acs@author@footnotes{}
                           683 \newcommand*\acs@author@list@main{%
                           684
                               \advance\@tempcnta\@ne\relax
                               \def\acs@author@footnotes{}%
                           685
                               \acs@author@list@and
                           686
                           687
                               \space
```

```
\acs@author@list@comma
                         689
                             \acs@author@star
                         690
                             \acs@author@affil
                         691
                             \acs@author@affil@also
                         692
                             \acs@author@affil@alt
                         693
                             \ifx\@empty\acs@author@footnotes\else
                         694
                                \textsuperscript{\acs@author@footnotes}%
                         695
                         696
                              \ifnum\@tempcnta<\acs@author@cnt\relax
                         697
                                \expandafter\acs@author@list@main
                         698
                             \fi
                         699
                        700 }
                         Simple checks to add an "and" and a comma.
  \acs@author@list@and
\acs@author@list@comma
                        701 \newcommand*\acs@author@list@and{%
                             \ifnum\acs@author@cnt=\@ne\relax\else
                         702
                                \ifnum\@tempcnta=\acs@author@cnt\relax
                         703
                                  \space and%
                         704
                                \fi
                         705
                         706
                             \fi
                         707 }
                         708 \newcommand*\acs@author@list@comma{%
                             \ifnum\acs@author@cnt>\tw@\relax
                                \ifnum\@tempcnta<\acs@author@cnt\relax
                         711
                                  ,%
                                \fi
                         712
                             \fi
                         713
                        714}
                        A check for an e-mail for an author: if so, add a star.
      \acs@author@star
  \acs@author@star@aux
                        715 \newcommand*\acs@author@star{%
                             \acs@ifundefined{@email@\@roman\@tempcnta}{}{%
                        716
                                \acs@author@star@aux
                         717
                        718
                             }%
                        719 }
                         720 \newcommand*\acs@author@star@aux{%
                              \protected@edef\acs@author@footnotes{%
                                \acs@author@fnsymbol{\z@}%
                        722
                                \ifnum\acs@affil@cnt>\@ne\relax
                        723
                                  ,%
                         724
                                \else
                         725
                                  \ifnum\acs@affil@alt@cnt>\z@\relax
                         726
                                    ,%
                         727
                        728
                                  \fi
                                \fi
                         729
                             }%
                        730
                         731 }
     \acs@author@affil The main affiliation of the author is checked for, and assuming one is found the
\acs@author@affil@aux appropriate symbol is added to the list.
                         732 \newcommand*\acs@author@affil{%
                            \acs@ifundefined{%
                               @affil@\@roman\csname @author@affil@\@roman\@tempcnta\endcsname
                         734
```

\@nameuse{@author@\@roman\@tempcnta}%

688

```
}{%
735
       \acs@warning{%
736
         No affiliation given for author\MessageBreak
737
         \@nameuse{@author@\@roman\@tempcnta}%
738
739
    }{%
740
       \acs@author@affil@aux
741
    }%
742
743 }
744 \newcommand*\acs@author@affil@aux{%
     \ifnum\acs@affil@cnt>\@ne\relax
745
       \expandafter\acs@affil@marker@cnt\csname @author@affil@\@roman
746
         \@tempcnta\endcsname\relax
747
       \advance\acs@affil@marker@cnt\acs@footnote@cnt\relax
748
       \protected@edef\acs@author@footnotes{%
749
         \acs@author@footnotes
750
         \acs@author@fnsymbol{\acs@affil@marker@cnt}%
751
       }%
752
     \else
753
       \ifnum\acs@affil@alt@cnt>\z@\relax
754
         \acs@affil@marker@cnt\@ne\relax
755
         \advance\acs@affil@marker@cnt\acs@footnote@cnt\relax
756
         \protected@edef\acs@author@footnotes{%
757
           \acs@author@footnotes
758
           \acs@author@fnsymbol{\acs@affil@marker@cnt}%
759
         }%
760
       \fi
761
    \fi
762
763 }
```

\acs@author@affil@also\acs@author@affil@also@aux

The "also" affiliations are generated by a loop as there may be more than one.

```
_{764} \ensuremath{\mbox{\sc Qauthor Qaffil Qalso}} \%
                      766
                                \acs@author@affil@also@aux
                    }%
767
768 }
_{769} \mbox{\ensuremath{\mbox{\sc Qauthor Qaffil Qalso Qaux}}} \%
                      \verb|\expandafter|@for| expandafter| @tempa| expandafter: | expandafter| | expanda
                                =\csname @author@alsoaffil@\@roman\@tempcnta\endcsname\do{%
771
                                 \acs@affil@marker@cnt\@tempa\relax
772
                                 \advance\acs@affil@marker@cnt\acs@footnote@cnt\relax
773
                                 \protected@edef\acs@author@footnotes{%
774
                                          \acs@author@footnotes
775
776
                                          \acs@author@fnsymbol{\acs@affil@marker@cnt}%
777
                                }%
778
                     }%
779
780 }
```

\acs@author@affil@alt \acs@author@affil@alt@aux Alternative affiliations get the correct affiliation number back out from the stored data. There are then two corrections: one for the total number of main affiliations and a second in case there is a footnote to the title.

```
781 \newcommand*\acs@author@affil@alt{\% 782 \acs@ifundefined{@author@altaffil@\@roman\@tempcnta}{}{\% 781 \newcommand*\acs@author@altaffil@\@roman\@tempcnta}
```

```
\acs@author@affil@alt@aux
783
          }%
784
785 }
786 \newcommand*\acs@author@affil@alt@aux{%
787
           \expandafter\acs@affil@marker@cnt
                \csname @author@altaffil@\@roman\@tempcnta\endcsname\relax
788
           \advance\acs@affil@marker@cnt\acs@affil@cnt\relax
789
           \advance\acs@affil@marker@cnt\acs@footnote@cnt\relax
790
            \protected@edef\acs@author@footnotes{%
791
                \acs@author@footnotes
792
                 ,%
793
                \acs@author@fnsymbol{\acs@affil@marker@cnt}%
794
          }%
795
796 }
The ACS have an extended list of symbols. The star appears at the special
position zero.
797 \newcommand*{\acs@author@fnsymbol}[1]{%
           \ensuremath{%
                 \expandafter\acs@author@fnsymbol@aux\expandafter{\number#1 }%
          }%
801 }
802 \mbox{ newcommand*{\acs@author@fnsymbol@aux}[1]{\%}}
           \ifnum#1>10 %
803
                \expandafter\acs@author@fnsymbol@loop
804
            \else
805
                \expandafter\acs@author@fnsymbol@symbol
806
807
            \fi
808
809 }
810 \mbox{ } \mbox{newcommand*{\acs@author@fnsymbol@loop}[1]{}}
             \acs@author@fnsymbol@loop@aux@i#1%
811
812 }
813 \neq 0 \newcommand*{\acs@author@fnsymbol@loop@aux@i}[2]{%
           \acs@author@fnsymbol@symbol{\ifnum#2=0 10\else #2\fi}\%
814
            \expandafter\acs@author@fnsymbol@loop@aux@ii\romannumeral #1000Q{}%
815
                 {\acs@author@fnsymbol@symbol{\ifnum#2=0 10\else #2\fi}}%
816
817 }
818 \mbox{ newcommand} {\acs@author@fnsymbol@loop@aux@ii}[1]{%}
            \@nameuse{acs@author@fnsymbol@loop@aux@#1}%
820 }
821 \def\acs@author@fnsymbol@loop@aux@m#1Q#2#3{%
           \label{loopQauxQii#1Q{#2#3}{#3}% The constant of the constan
822
823 }
824 \mbox{newcommand} {\acs@author@fnsymbol@loop@aux@Q}[2]{#1}
825 \newcommand*{\acs@author@fnsymbol@symbol}[1]{%
826
           \ifcase #1 *\or
827
                \dagger\or
                     \ddagger\or
828
                          \P\or
829
                               \S\or
```

\acs@author@fnsymbol \acs@author@fnsymbol@aux

831

832

833

\|\or \bot\or

\#\or

\acs@author@fnsymbol@loop

cs@author@fnsymbol@loop@aux@i

s@author@fnsymbol@loop@aux@ii

cs@author@fnsymbol@loop@aux@m

cs@author@fnsymbol@loop@aux@Q

\acs@author@fnsymbol@symbol

\acs@address@list
\acs@address@list@auxi
\acs@address@list@auxii

Loop over the addresses and any extra affiliations and print them all: if there is only one, omit the marker entirely. There is also a need to watch out for any footnotes from the title.

```
839 \newcommand*\acs@address@list{%
    \ifnum\acs@affil@cnt>\z@
840
       \expandafter\acs@address@list@auxi
841
842
     \else
       \acs@warning{No affiliations: at least one affiliation is needed}%
843
844
    \fi
845 }
846 \newcommand*\acs@address@list@auxi{%
    \ifnum0%
848
       \ifnum\acs@affil@cnt>\@ne
       \ifnum\acs@affil@alt@cnt>\z@ 1\fi
849
850
       \expandafter\acs@address@list@auxii
851
     \else
852
       \@address@i\par
853
854
855 }
856 \newcommand*\acs@address@list@auxii{%
     \@tempcnta\z@
     \acs@affil@marker@cnt\acs@footnote@cnt
858
     \loop\ifnum\@tempcnta<\acs@affil@cnt
859
       \advance\@tempcnta\@ne
860
       \advance\acs@affil@marker@cnt\@ne
861
       \acs@author@fnsymbol{\acs@affil@marker@cnt}%
862
       \@nameuse{@address@\@roman\@tempcnta}\par
863
     \repeat
864
     \@tempcnta\z@
865
     \loop\ifnum\@tempcnta<\acs@affil@cnt
866
       \advance\@tempcnta\@ne
867
868
       \advance\acs@affil@marker@cnt\@ne
       \acs@ifundefined{@altaffil@\@roman\@tempcnta}
869
870
         {}
         {%
871
           \acs@author@fnsymbol{\acs@affil@marker@cnt}%
872
           \@nameuse{@altaffil@\@roman\@tempcnta}\par
873
874
875
     \repeat
876 }
```

\acs@fnsymbol@org \acs@affil@list \acs@affil@list@aux Footnotes are done in two stages. First the main affiliation is handled, then the possible alternative. There is a need to check for the possibility that there is only one main affiliation but one or more alternative ones.

```
877 \newcommand*\acs@fnsymbol@org{}
878 \newcommand*\acs@affil@list{%
879 \let\acs@fnsymbol@org\@fnsymbol
```

```
\@tempcnta\z@\relax
                           881
                                \@tempcntb\z@\relax
                           882
                                \ifnum\acs@affil@cnt>\@ne\relax
                           883
                                  \expandafter\acs@affil@list@aux
                           884
                                \else
                           885
                                  \ifnum\acs@affil@alt@cnt>\z@\relax
                           886
                                    \acs@affil@marker@cnt\@ne\relax
                           887
                                    \advance\acs@affil@marker@cnt\acs@footnote@cnt\relax
                           888
                                    \footnotetext[\acs@affil@marker@cnt]{\@affil@i}%
                           889
                                    \@tempcnta\@ne\relax
                           890
                                  \fi
                           891
                                \fi
                           892
                                \ifnum\acs@affil@alt@cnt>\z@\relax
                           893
                                  \expandafter\acs@affil@alt@list
                           894
                                \fi
                           895
                                \let\@fnsymbol\acs@fnsymbol@org
                           896
                           897 }
                           898 \newcommand*\acs@affil@list@aux{%
                                \advance\@tempcnta\@ne\relax
                           899
                                \acs@affil@marker@cnt\@tempcnta\relax
                                \advance\acs@affil@marker@cnt\acs@footnote@cnt\relax
                                \footnotetext[\acs@affil@marker@cnt]{%
                           902
                                  \@nameuse{@affil@\@roman\@tempcnta}%
                           903
                                }%
                           904
                                \ifnum\@tempcnta<\acs@affil@cnt\relax
                           905
                                  \expandafter\acs@affil@list@aux
                           906
                                \fi
                           907
                           908 }
     \acs@affil@alt@list
                           The secondary loop for alternative affiliations is similar.
\acs@affil@alt@lista@aux
                          909 \newcommand*\acs@affil@alt@list{%
                                \advance\@tempcntb\@ne\relax
                                \acs@ifundefined{@altaffil@\@roman\@tempcntb}{}{%
                                  \acs@altaffil@foot@aux
                           912
                               }
                           913
                                \ifnum\@tempcntb<\acs@author@cnt\relax
                           914
                                  \expandafter\acs@affil@alt@list
                           915
                           916
                           917 }
                           918 \newcommand*\acs@altaffil@foot@aux{%
                                \advance\@tempcnta\@ne\relax
                           919
                                \acs@affil@marker@cnt\@tempcnta\relax
                                \advance\acs@affil@marker@cnt\acs@footnote@cnt\relax
                                \footnotetext[\acs@affil@marker@cnt]{%
                                  \@nameuse{@altaffil@\@roman\@tempcntb}%
                           923
                                }%
                           924
                           925 }
    \acs@email@list@font
```

\let\@fnsymbol\acs@author@fnsymbol

880

\acs@email@list@font \acs@email@list \acs@email@list@aux The final piece of meta-data to print is the e-mail address list. The total number of e-mail addresses given it counted in \@tempcntb, which means a warning can be given if there are none. The group is used so that \UrlFont can be set correctly.

926 \newcommand\*\acs@email@list@font{\sf}

```
927 \newcommand*\acs@email@list{%
    \begingroup
928
       \def\UrlFont{\acs@email@list@font}%
929
       \@tempcnta\z@\relax
930
       \@tempcntb\z@\relax
931
       \acs@email@list@aux
932
       \ifnum\@tempcntb=\z@\relax
933
         \acs@warning{%
934
           No e-mail given:\MessageBreak
935
           at lest one author must have a contact e-mail%
936
         }%
937
       \fi
938
     \endgroup
939
940 }
941 \neq 0 \newcommand*\acs@email@list@aux{%
     \advance\@tempcnta\@ne\relax
942
     \ifnum\@tempcnta>\acs@author@cnt\relax\else
943
       \acs@ifundefined{@email@\@roman\@tempcnta}{}{%
944
         \advance\@tempcntb\@ne\relax
945
         \ifnum\@tempcntb>\@ne\relax
946
947
         \fi
948
         \expandafter\expandafter\expandafter\url\expandafter
949
           \expandafter\expandafter{%
950
               \csname @email@\@roman\@tempcnta\endcsname
951
         }%
952
       }%
953
       \expandafter\acs@email@list@aux
954
955
956 }
```

\acs@number@list \acs@number@list@aux@i \acs@number@list@aux@ii Listing phone and fax numbers is easier as they don't have to be given. Everything is done in one block so that it is possible to know whether to add a new line and also to keep everything together.

```
957 \newcommand*\acs@number@list{%
    \begingroup
958
       \acs@number@list@aux@i{phone}%
959
       \let\@tempb\@tempa
960
       \acs@number@list@aux@i{fax}%
961
       \ifx\@tempa\@empty
962
         \let\@tempa\@tempb
963
964
       \else
         \ifx\@tempb\@empty\else
965
966
           \protected@edef\@tempa{%
              \@tempb.\space\@tempa
967
           }%
968
         \fi
969
       \fi
970
       \ifx\@tempa\@empty\else
971
         \par
972
         \@tempa
973
974
     \endgroup
975
976 }
```

```
\def\@tempa{}%
                               978
                                    \@tempcnta\z@\relax
                               979
                                    \def\acs@number@list@aux@ii{%
                               980
                                      \advance\@tempcnta\@ne\relax
                               981
                               982
                                      \ifnum\@tempcnta>\acs@author@cnt\relax\else
                               983
                                         \acs@ifundefined{@#1@\@roman\@tempcnta}{}{%
                               984
                                           \acs@ifundefined{@email@\\email@\\eman\\@tempcnta}{}{%
                               985
                                             \ifx\@tempa\@empty
                                               \edef\@tempa{%
                               986
                                                 \@nameuse{@#1@\@roman\@tempcnta}%
                               987
                                               }%
                               988
                                             \else
                               989
                                               \edef\@tempa{%
                               990
                                                 \@tempa
                               991
                               992
                                                  \@nameuse{@#1@\@roman\@tempcnta}%
                               993
                                               }%
                               994
                                             \fi
                               995
                                          }%
                               996
                                        }%
                               997
                                         \expandafter\acs@number@list@aux@ii
                               998
                                      \fi
                               999
                                    }%
                              1000
                                    \acs@number@list@aux@ii
                              1001
                                    \ifx\@tempa\@empty\else
                              1002
                                      \protected@edef\@tempa{%
                              1003
                                         \MakeUppercase#1: \@tempa
                              1004
                                      }%
                              1005
                              1006
                                    \fi
                              1007 }
                              1008 \newcommand*\acs@number@list@aux@ii{}
               \endabstract
      \verb|\acs@abstract@extras||_{1009} \verb|\g@addto@macro|| endabstract{%}
                                    \aftergroup\acs@abstract@extras
                              1011 }
                              1012 \newcommand*{\acs@abstract@extras}{%
                                   \ifacs@abbreviations
                              1013
                                      \acs@abbreviations@print
                              1014
                                      \par
                              1015
                                    \fi
                              1016
                                    \ifacs@keywords
                              1017
                                      \acs@keywords@print
                              1018
                              1019
                                    \fi
                              1020
                              1021 }
     \acs@maketitle@extras A couple of things might need to be added to \maketitle.
\verb|\acs@maketitle@extras@hook||_{1022} \verb|\newcommand*| acs@maketitle@extras{\%|}|
                                    \acs@maketitle@extras@hook
                              1023
                              1024 }
                              1025 \newcommand*\acs@maketitle@extras@hook{}
                              1026 \g@addto@macro{\maketitle}{\acs@maketitle@extras}
```

977 \newcommand\*\acs@number@list@aux@i[1]{%

```
variation is allowed, and so it is done automatically.
                        1027 \g@addto@macro{\document}{\maketitle}
                 scheme
                        Three new float types are provided, scheme, chart and graph. These are the
                 chart most obvious types; for graphs, a slight problem arises with the file extension.
                 graph 1028 \newfloat{scheme}{htbp}{los}
                        1029 \floatname{scheme}{Scheme}
                        1030 \newfloat{chart}{htbp}{loc}
                        1031 \floatname{chart}{Chart}
                        1032 \newfloat{graph}{htbp}{loh}
                        1033 \floatname{graph}{Graph}
           \schemename Naming is set up in the same way as the kernel floats.
            \chartname 1034 \newcommand*\schemename{Scheme}
            \graphname 1035 \newcommand*\chartname{Chart}
                        1036 \newcommand*\graphname{Graph}
                        The standard floats should appear "here" by default.
                        1037 \floatplacement{table}{htbp}
                        1038 \floatplacement{figure}{htbp}
                        1039 \floatstyle{plaintop}
                        1040 \restylefloat{table}
    \acs@floatboxreset Floats are all centred.
                        1041 \let\acs@floatboxreset\@floatboxreset
                        1042 \def\@floatboxreset{%
                        1043 \centering
                        1044
                             \acs@floatboxreset
                        1045 }
             \plainref For legacy support.
                  \ref 1046 \newcommand*\plainref{}
                        1047 \AtBeginDocument{\let\plainref\ref}
          \acs@section Both the numbering and existence of section headers may need to be altered.
       \acs@subsection Some generic functions are therefore provided to deal with this cleanly. First,
    \acs@subsubsection some original definitions are saved.
\verb|\acs@startsection@orig||_{1048} \verb|\newcommand*\acs@section{}|
                        1049 \let\acs@section\section
                        1050 \newcommand*\acs@subsection{}
                        1051 \let\acs@subsection\subsection
                        1052 \newcommand*\acs@subsubsection{}
                        1053 \let\acs@subsubsection\subsubsection
                        1054 \newcommand*\acs@startsection@orig{}
                        1055 \let\acs@startsection@orig\@startsection
     \acs@startsection A version of \@startsection which adds unnumbered sections to the TOC:
                         modelled on amsart. This is active as standard.
                        1056 \newcommand\acs@startsection[6]{%
```

1057 \if@noskipsec \leavevmode \fi
1058 \par \@tempskipa #4\relax

\maketitle is required by the document class, and must start the document. No

```
1059 \@afterindenttrue
                                                  1060 \ifdim \@tempskipa <\z@ \@tempskipa -\@tempskipa \@afterindentfalse\fi
                                                           \if@nobreak \everypar{}\else
                                                                     \addpenalty\@secpenalty\addvspace\@tempskipa\fi
                                                  1062
                                                           \c \fi = \c \fi
                                                  1063
                                                                             {\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}
                                                  1064
                                                  1066 \let\@startsection\acs@startsection
  \acs@startsection@alt An alternative version of \@startsection which never adds numbers.
                                                  1067 \newcommand*\acs@startsection@alt[6]{%
                                                             \if@noskipsec \leavevmode \fi
                                                             \par \@tempskipa #4\relax
                                                            \@afterindenttrue
                                                  1070
                                                  1071 \ifdim \@tempskipa <\z@ \@tempskipa -\@tempskipa \@afterindentfalse\fi
                                                  1072 \if@nobreak \everypar{}\else
                                                                    \addpenalty\@secpenalty\addvspace\@tempskipa\fi
                                                              \c \fi = {4}{\#5}{\#6}
                                                                               {\@ssect{#3}{#4}{#5}{#6}}%
                                                  1075
                                                  1076 }
        \acs@sections@none When removing sections entirely, a gobble macro is needed.
\verb|\acs@sections@none@aux| $_{1077} \le \text{mewcommand*} \ acs@sections@none{\%} |
                                                  1078
                                                             \@ifstar{%
                                                                  \acs@sections@none@aux
                                                  1079
                                                  1080
                                                  1081
                                                                  \acs@sections@none@aux
                                                  1082
                                                  1083 }
                                                  1084 \newcommand*\acs@sections@none@aux[2][]{%
                                                              \acs@warning{%
                                                  1085
                                                                   (Sub)section '#2' ignored%
                                                  1086
                                                  1087
                                                  1088 }
                                                   To macros to add or remove the section numbers. The standard setting for the
        \SectionNumbersOff
                                                   class has them on, but some configurations will turn them off. The names of
           \SectionNumbersOn
                                                     these functions are both in design space so that users can change the decision
                                                    easily.
                                                  1089 \newcommand*\SectionNumbersOff{%
                                                             \let\@startsection\acs@startsection@alt
                                                  1090
                                                  1091 }
                                                  1092 \@onlypreamble\SectionNumbersOff
                                                  1093 \newcommand*\SectionNumbersOn{%
                                                             \let\@startsection\acs@startsection
                                                  1094
                                                  1095 }
                                                  1096 \@onlypreamble\SectionNumbersOn
                      \SectionsOff Quite similar for entire sections.
                        \verb|\SectionsOn|_{1097} \verb|\newcommand*| SectionsOff{\%}
                                                  1098
                                                            \let\section\acs@sections@none
                                                             \let\subsection\acs@sections@none
```

\let\subsubsection\acs@sections@none

```
1101 }
                       1102 \@onlypreamble\SectionsOff
                       1103 \newcommand*\SectionsOn{%
                            \let\section\acs@section
                            \let\subsection\acs@subsection
                       1105
                            \let\subsubsection\acs@subsubsection
                       1108 \@onlypreamble\SectionsOn
     \tableofcontents Never print TOC in itself.
                       1109 \begingroup
                            \toks@=\expandafter{\tableofcontents}
                            \xdef\tableofcontents{%
                       1112
                               \begingroup
                                 \let\noexpand\@startsection\noexpand\acs@startsection@orig
                       1113
                       1114
                       1115
                              \endgroup
                       1116
                       1117 \endgroup
      acknowledgement Simple named sections.
             suppinfo 1118 \newenvironment{acknowledgement}{%
                       1119 \acs@section*{\acknowledgementname}%
                       1120 }{}
                       1121 \newenvironment{suppinfo}{%
                       1122 \acs@section*{\suppinfoname}%
                       1123 }{}
 \acknowledgementname A few macros need to get around the changes.
          \verb|\bibsection|_{1124} \verb|\newcommand*| acknowledgementname{Acknowledgement}|
        \suppinfoname 1125 \AtEndOfClass{%
                       1126 \def\bibsection{%
                              \verb|\acs@section*{\refname}||%
                       1127
                            }%
                       1128
                       1129}
                       1130 \newcommand*\suppinfoname{Supporting Information Available}
        \acs@abstract Removing the abstract, if necessary, is done using a trick from the comment
     \acs@endabstract package. However, it code is copied here to keep requirements down.
  \acs@abstract@start 1131 \newcommand*\acs@abstract{}
    \acs@abstract@end 1132 \let\acs@abstract\abstract
\acs@abstract@iffalse 1133 \newcommand*\acs@endabstract{}
                       1134 \let\acs@endabstract\endabstract
                       1135 \begingroup
                       1136 \catcode'{ \active
                           \catcode'} 12\relax
                       1137
                       1138 \catcode'( 1\relax
                       1139 \catcode') 2\relax
                       1140 \gdef\acs@abstract@start(%
                              \acs@warning(%
                       1141
                                Abstract not allowed for this\MessageBreak
                       1142
                                 manuscript type
                       1143
                              )%
                       1144
                              \@bsphack
                       1145
```

```
\catcode'} 12\relax
                     1147
                             \let\end\fi
                     1148
                             \let{\acs@abstract@end% }
                     1149
                            \iffalse
                     1150
                          )%{
                     1151
                           \gdef\acs@abstract@end#1}(%
                     1152
                             \def\@tempa(#1)\%
                     1153
                             \ifx\@tempa\@currenvir
                     1154
                               \@Esphack\endgroup
                     1155
                               \if@ignore
                     1156
                                 \global\@ignorefalse
                     1157
                                 \ignorespaces
                     1158
                               \fi
                     1159
                             \else
                     1160
                                \expandafter\acs@abstract@iffalse
                     1161
                     1162
                          )
                     1163
                     1164 \endgroup
                     1165 \newcommand*\acs@iffalse{\iffalse}
        \AbstractOff A very similar pattern to before.
         \AbstractOn 1166 \newcommand*\AbstractOff{%
                     1167
                          \let\abstract\acs@abstract@start
                     1168
                          \let\endabstract\acs@abstract@end
                     1169 }
                     1170 \@onlypreamble\AbstractOff
                     1171 \newcommand*\AbstractOn{%
                          \let\abstract\acs@abstract
                     1172
                          \let\endabstract\acs@endabstract
                     1173
                     1174 }
                     1175 \@onlypreamble\AbstractOn
                      The content of the graphic TOC entry is processed using a method from amsmath
   \acs@collect@toks
\acs@collect@content
                      via environ. The entire environment is gathered for typesetting in a box. First,
                      some storage is needed.
\acs@collect@content
                     1176 \newtoks\acs@collect@toks
                     1177 \newtoks\acs@collect@empty@toks
                     1178 \newcommand*\acs@collect@begins{}
                     1179 \newcommand*\acs@collect@content{}
        \acs@collect This is a \long version of \collect@body.
   \acs@collect@begins@ 1181
                          \acs@collect@toks{%
                            \expandafter#1\expandafter{\the\acs@collect@toks}%
   \acs@collect@body 1182
                     1183 }%
                          \edef\acs@collect@content{%
                            \the\acs@collect@toks
                     1185
                     1186
                            \noexpand\end{\@currenvir}%
                     1187
                          \acs@collect@toks\acs@collect@empty@toks
                     1188
                          \def\acs@collect@begins{b}%
                     1189
                          \begingroup
                     1190
                             \expandafter\let\csname\@currenvir\endcsname\acs@collect@aux
                     1191
```

\catcode'{ \active

1146

```
\edef\acs@collect@content{%
1192
          \expandafter\noexpand\csname\@currenvir\endcsname
1193
        }%
1194
        \acs@collect@content
1195
1196 }
1197 \newcommand*\acs@collect@aux{}
1198 \long\def\acs@collect@aux#1\end#2{%
      \edef\acs@collect@begins{%
        \acs@collect@begins@#1\begin\end
        \expandafter\@gobble\acs@collect@begins
1201
     }%
1202
      \ifx\@empty\acs@collect@begins
1203
        \endgroup
1204
        \c0checkend{#2}%
1205
        \acs@collect@body{#1}%
1206
      \else
1207
        \acs@collect@body{\#1\end{\#2}}\%
1208
      \fi
1209
      \acs@collect@content
1211 }
1212 \newcommand*\acs@collect@begins@{}
{\tt 1213 \ long\ def\ acs@collect@begins@#1\ begin#2{\%}}
     \ifx\end#2\else
1214
        b\expandafter\acs@collect@begins@
1215
1216
     \fi
1217 }
1218 \newcommand\acs@collect@body[1] {%
      \global\acs@collect@toks\expandafter{\the\acs@collect@toks#1}%
```

\acs@abstract@print

Delayed abstract printing works in a similar way, but with some formatting 'built-in'.

```
1221 \newcommand\acs@abstract@print[1]{%
      \global\long\def\acs@abstract@text{%
1222
        \if@twocolumn
1223
          \@restonecoltrue\onecolumn
1224
1225
          \@restonecolfalse\newpage
1226
        \fi
1227
        \acs@section*{Abstract}%
1228
        #1%
1229
        \if@restonecol
1230
          \twocolumn
1231
        \else
1232
          \newpage
1233
1234
1235
      \AtEndDocument{\acs@abstract@text}%
1236
```

\acs@tocentry@print

The same approach is taken for the graphical table of content printing. This is \acs@tocentry@print@aux done in a box so that everything has a frame around it.

```
\acs@tocentry@text 1238 \newcommand{\acs@tocentry@print}[1]{%
                       \gdef\acs@tocentry@text{\normalsize#1}%
```

```
\if@twocolumn
                  1241
                            \@restonecoltrue\onecolumn
                  1242
                          \else
                  1243
                            \@restonecolfalse\newpage
                  1244
                  1245
                          \acs@tocentry@print@aux
                  1246
                          \if@restonecol
                  1247
                            \twocolumn
                  1248
                          \else
                  1249
                            \newpage
                  1250
                          \fi
                  1251
                       }%
                  1252
                  1253 }
                  1254 \newcommand*{\acs@tocentry@print@aux}{%
                        \begingroup
                  1255
                          \let\@startsection\acs@startsection@orig
                  1256
                          \acs@section*{\tocentryname}%
                  1257
                  1258
                          \tocsize
                          \sffamily
                  1259
                          \singlespacing
                  1260
                          \begin{center}
                  1261
                            \fbox
                  1262
                              {%
                  1263
                                \begin{minipage}{\acs@tocentry@height}
                  1264
                                  \vbox to \acs@tocentry@width{\acs@tocentry@text}%
                  1265
                                \end{minipage}%
                  1266
                              }%
                  1267
                          \end{center}%
                  1268
                  1269
                        \endgroup
                  1270 }
                  1271 \newcommand*\acs@tocentry@text{TOC ENTRY REQUIRED}
                  1272 \newlength{\acs@tocentry@height}
                  1273 \newlength{\acs@tocentry@width}
                  1274 \setlength{\acs@tocentry@height}{9 cm}
                  1275 \setlength{\acs@tocentry@width}{3.5 cm}
         tocentry Actually creating the entry is pretty easy.
                  \tocentryname A simple name macro.
                  1277 \newcommand*\tocentryname{Graphical TOC Entry}
         \tocsize The font size for printing the TOC entry.
                  1278 \newcommand*\tocsize{%
                       \@setfontsize\tocsize\@viiipt\@ixpt
                  1279
                  1280 }
  \acs@type@list Different journals allow different types of article. A list is set up here: different
                  journals can then alter it. A check function is also provided along with a default.
\acs@type@default
 \acs@type@check 1281 \newcommand*\acs@type@list{article,communication,suppinfo}
                  1282 \newcommand*\acs@type@default{article}
                  1283 \newcommand*\acs@type@check{%
                  1284 \@tempswafalse
```

\AtEndDocument{%

1240

```
\ifx\@tempa\acs@manuscript
                    1286
                              \expandafter\@tempswatrue
                    1287
                    1288
                            \fi
                         }%
                    1289
                          \if@tempswa\else
                    1290
                            \acs@warning{%
                    1291
                              Invalid manuscript type \acs@manuscript:\MessageBreak
                    1292
                              changed to default type \acs@type@default
                    1293
                            }%
                    1294
                            \let\acs@manuscript\acs@type@default
                    1295
                          \fi
                    1296
                    1297 }
                        A few bits for older versions.
                    1298 \newcommand*\acs@setkeys{\setkeys{acs}}
                    1299 \let\acs@killabstract\AbstractOff
                    1300 \let\acs@killsecs\SectionsOff
                    1301 \newcommand*\acs@validtype[2][article]{%
                         \def\acs@type@default{#1}%
                          \def\acs@type@list{#2}%
                    1304 }
          \acs@par A saved paragraph.
                    1305 \newcommand*\acs@par{}
                    1306 \let\acs@par\par
\acs@layout@shared Some code is used generally when setting up "press ready" layouts. There is
   acknowledgement
                     quite a bit here, mainly layout related.
          suppinfo 1307 \newcommand*\acs@layout@shared{%
                         \AtBeginDocument{\singlespacing}%
                    1308
                          \twocolumn
                    1309
                          \tolerance=2000\relax
                    1310
                          \emergencystretch=10pt\relax
                    1311
                          \geometry{
                    1312
                            letterpaper,
                    1313
                            top
                                  = 12.7 mm
                    1314
                            bottom = 16.8mm,
                    1315
                            left = 19.3mm,
                    1316
                           right = 19.3mm
                    1317
                         }%
                    1318
                          \setlength{\columnsep}{8.1mm}%
                    1319
                          \setlength{\parindent}{3.3mm}%
                    1320
                          \renewenvironment{acknowledgement}{%
                    1321
                            \def\@tempa{acknowledgement}%
                    1322
                            \ifx\@currenvir\@tempa
                    1323
                              \let\par\relax
                    1324
                              \acksize
                    1325
                    1326
                              \vspace{6pt}%
                              \textbf{\acknowledgementname}%
                    1327
                    1328
                              \acs@section*{\acknowledgementname}%
                    1329
                            \fi
                    1330
                         }{%
                    1331
```

 $\label{lem:condition} $$ \ensuremath{\tt 0for\@tempa:=\acs@type@list\do{\%} } $$$ 

1285

```
\acs@par
                 1332
                 1333 }%
                 1334 }
        \acksize More sizes.
       \suppsize 1335 \newcommand*\acksize{\normalsize}
                 1336 \newcommand*\suppsize{\normalsize}
\acs@layout@nine The class loads twelve point text. To reset it for print layouts, it is easiest to do
          \@xipt things directly.
 \label{lagrange} $$\acs@layout@ten_{1337} \rightarrow \acs@layout@nine{\%} $$
                 1338
                       \def\@xipt{11}%
                       \long\def\normalsize{%
                 1339
                        \@setfontsize\normalsize\@ixpt\@xipt
                 1340
                 1341
                 1342
                       \normalsize
                       \let\@listi\@listI
                       \abovedisplayskip 5\p@ \@plus2\p@ \@minus 5\p@\relax
                       \abovedisplayshortskip \z@ \@plus3\p@\relax
                       \belowdisplayshortskip 3\p@ \@plus3\p@ \@minus 3\p@\relax
                 1346
                       \belowdisplayskip\abovedisplayskip\relax
                 1347
                       \abovecaptionskip 5\p@\relax
                 1348
                       \intextsep 7\p0 \@plus 2\p0 \@minus 2\p0\relax
                 1349
                 1350 }
                 1351 \newcommand*\acs@layout@ten{%
                       \long\def\normalsize{%
                         \@setfontsize\normalsize\@xpt\@xiipt
                 1353
                 1354 }%
                 1355 \normalsize
                 1356 \@setfontsize\normalsize\@xpt\@xiipt
                 1357 \let\@listi\@listI
                       \abovedisplayskip 10\p@ \@plus2\p@ \@minus5\p@\relax
                 1358
                       \abovedisplayshortskip \z@ \@plus3\p@\relax
                 1359
                       \belowdisplayshortskip 6\p0 \@plus3\p0 \@minus3\p0\relax
                 1360
                       \belowdisplayskip \abovedisplayskip\relax
                 1361
                 1362 }
                      With all of the standard settings done, the journal configuration can be
                  loaded.
                 1363 \InputIfFileExists{achemso-\acs@journal.cfg}{}{%
                       \acs@warning{%
                 1364
                         Unknown journal '\acs@journal':\MessageBreak
                 1365
                         using default configuration JACSAT%
                 1366
                       ጉ%
                 1367
                       \input{achemso-jacsat.cfg}%
                 1368
        \thepage Some changes that can always be applied if the manuscript type is appropriate:
                   this saves some repetition in the configuration files.
                 1370 \acs@type@check
                 1371 \ifx\acs@manuscript\acs@manuscript@note
                 1372 \SectionsOff
```

1373 \fi

```
{\tt 1374} \verb|\ifx\acs@manuscript\acs@manuscript@review|
      \SectionsOn
1375
      \SectionNumbersOn
1376
1377\fi
1378 \ifx\acs@manuscript\acs@manuscript@suppinfo
      \setkeys{acs}{maxauthors = 0}
1379
      \def\thepage{S-\arabic{page}}
1380
      \renewcommand*\thefigure{S\@arabic\c@figure}
1381
      \renewcommand*\thescheme{S\@arabic\c@scheme}
      \renewcommand*\thetable{S\@arabic\c@table}
      \AtBeginDocument
1384
        ₹%
1385
           \renewcommand*\citenumfont[1]{S#1}%
1386
          \renewcommand*\bibnumfmt[1]{(S#1)}%
1387
1388
1389\fi
    Set up two column layout.
1390 \begingroup
      \def\@tempa{twocolumn}
1391
      \ifx\acs@layout\@tempa
1392
        \aftergroup\acs@layout@shared
1393
      \fi
1394
      \def\@tempa{two-column}
1395
      \ifx\acs@layout\@tempa
1396
        \aftergroup\acs@layout@shared
1397
      \fi
1398
1399 \endgroup
_{1400}\left</\mathsf{class}\right>
```

## 8.5 Late shared code

\citenumfont

Changes to citations can now be made. The citation styles supplied here require natbib, which is loaded with the appropriate options. This part applies to the package as well as the class: it is here so that the load order is correct.

```
1401 (*class | package)
1402 \ifacs@super
1403
     \RequirePackage[sort&compress,numbers,super]{natbib}
1404 \else
     \RequirePackage[sort&compress,numbers,round]{natbib}
1406
     \def\citenumfont{\textit}
1407\fi
1408 \define@key{acs}{super}[true]{%
     \def\@tempa{#1}%
1409
      \def\@tempb{true}%
1410
      \ifx\@tempa\@tempb
1411
        \setcitestyle{super,open={},close={}}%
1412
        \renewcommand*\citenumfont{}%
1413
1414
        \setcitestyle{round}%
1415
1416
        \renewcommand*\citenumfont{\textit}
1417
     \fi
1418 }
```

```
1419 \RequirePackage{natmove}
```

The mciteplus package allows the construction of lists of references with subletters. However, it might not be available, and so it is only loaded if available: the .bst files should work either way. There is also a patch to get crossreferences correct with the modified \ref macro used here. The reason for ensuring that \@mciteNatbibCiteCmdList is defined is that it allows for the case where people prevent mciteplus being loaded using \ver@mciteplus.sty.

```
1420 \IfFileExists{mciteplus.sty}{%
                                  \RequirePackage{mciteplus}
                                  \verb|\providecommand*{\cmciteNatbibCiteCmdList}{}|% \cline{Continuous continuous continuo
1422
                                  \edef\@tempa{\noexpand\in@{citenum}{\@mciteNatbibCiteCmdList}}%
1423
                                 \@tempa
1424
                                 \ifin@
1425
                                  \else
1426
                                            \edef\@mciteNatbibCiteCmdList{\@mciteNatbibCiteCmdList,citenum}%
1427
1428
                              \fi
1429 (*!package)
                                  \def\@mciteSubRef[##1]##2{\plainref{\@mcitereflabelprefix:##1:##2}}
1431 (/!package)
1432 }{}
```

\acs@bibstyle The next step is to sort out bibliography formatting. With both the package and the class, the bibliography style is determined without user intervention. The style is stored as it may need to be altered later.

```
1433 \newcommand*\acs@bibstyle{achemso}
1434 \ifacs@biochem
     \def\acs@bibstyle{biochem}
     \bibliographystyle{biochem}
1437 \else
1438 \bibliographystyle{achemso}
1439\fi
```

\acs@bibliographystyle The original \bibliographystyle macro is now disabled: the underlying com-\bibliographystyle mand is repeated otherwise problems cop up with chapterbib.

```
1440 \newcommand*\acs@bibliographystyle{}
1441 \let\acs@bibliographystyle\bibliographystyle
1442 \def\bibliographystyle#1{%
     \acs@warning{\string\bibliographystyle\space ignored}%
     \expandafter\acs@bibliographystyle\expandafter{\acs@bibstyle}%
1445 }
1446 (/class | package)
```

## Late package-only code

The notes2bib code may or may not be activated.

```
1447 (*package)
1448 \AtBeginDocument{%
      \@ifpackageloaded{notes2bib}{}{%
         \acs@niib@create
1450
      }%
1451
1452 }
_{1453}\left</\,\mathsf{package}\right>
```

## 8.7 Moving citations with natbib

The code for moving citations is created as a separate package, as the code needed is the same in both cases.

```
_{1454} \langle *natmove \rangle
1455 \ProvidesPackage{natmove}
1456 [2010/01/15 v1.1a Automatic citation moving with natbib]
1457 \RequirePackage{natbib}
```

\nmv@ifmtarg To keep down dependence on other packages, the very short code block from \nmv@xifmtarg ifmtarg is copied here with an internal name.

```
1458 \newcommand*\nmv@ifmtarg{}
1459 \newcommand*\nmv@xifmtarg{}
1460 \begingroup
1461 \catcode'\Q 3\relax
                                      \long\gdef\nmv@ifmtarg#1{%
1462
                                                                      \nmv@xifmtarg#1QQ\@secondoftwo\@firstoftwo\@nil
1463
1464 }
1465 \quad \label{eq:constraint} $$1465 \quad \label{eq:constraint} 
1466 \endgroup
```

\ifnmv@cite A flag is need to watch whether \cite or another macro is in use.

```
1467 \newif\ifnmv@cite
```

\nmv@citex Using the flag, either the new internal macro, or the natbib original, can be called.

```
1468 \newcommand*\nmv@citex{%
1469 \ifnmv@cite
       \expandafter\nmv@citex@moving
    \else
       \expandafter\nmv@citex@nat
1472
     \fi
1473
1474 }
```

\nmv@after Later, the argument for \cite will need to be saved.

```
1475 \newcommand*\nmv@after{}
```

\nmv@citex@moving

The new version of \@citex is needed that looks ahead of the citation using \futurelet. There are three arguments to \@citex when using natbib. Other than that, the trick used here is similar to that in cite.

```
1476 \newcommand*\nmv@citex@moving{}
1477 \def\nmv@citex@moving[#1][#2]#3{%
1478 \leavevmode
1479 \skip@\lastskip\relax
    \unskip
1480
1481 \begingroup
      1482
      \global\nmv@citefalse
1483
      \nmv@citex@get@next\relax
1484
1485 }
```

\nmv@citex@end To get things right at the end.

```
1486 \newcommand*\nmv@citex@end{%
       \nmv@after
1487
```

```
1488
     \endgroup
1489 }
```

\nmv@citex@get@next \nmv@citex@next

The next token on the input stack is saved into \nmv@citex@next, after gobbling up one token.

```
1490 \newcommand*\nmv@citex@get@next[1]{%
     \futurelet\nmv@citex@next\nmv@citex@punct
1492 }
```

\nmv@citex@punct \nmv@citex@punct@undouble \nmv@citex@loop

The working macro for moving the punctuation. This is very much like \@citey in the cite package. The initial assumption is that the loop will terminate, and so the recursion call will simply do the finalisation.

```
1493 \newcommand*\nmv@citex@punct{%
     \let\nmv@citex@loop\nmv@citex@end
     \ifx\nmv@citex@next.\relax
       \ifnum\spacefactor<\nmv@citex@sfac\else
1496
         \expandafter\expandafter\nmv@citex@punct@undouble
1497
1498
1499
     \expandafter\nmv@citex@punct@aux\natmovechars\@nil
1500
     \nmv@citex@loop
1501
1502 }
1503 \newcommand*\nmv@citex@punct@undouble{%
     \let\nmv@citex@next\relax
     \let\nmv@citex@loop\nmv@citex@get@next
1506}
1507 \newcommand*\nmv@citex@loop{}
```

\nmv@citex@punct@aux The final part of the punctuation moving system.

```
1508 \newcommand*\nmv@citex@punct@aux[1]{%
     \ifx\nmv@citex@next#1\@empty
1510
       #1%
        \let\nmv@citex@loop\nmv@citex@get@next
1511
1512
     \ifx#1\@nil\else
1513
       \expandafter\nmv@citex@punct@aux
1514
     \fi
1515
1516}
```

1527\fi

\nmv@citex@sfac The value of the spacing factor after a full stop is used to signal doubled punctuation. For French spacing, a bit of patching is needed.

```
1517 \mathchardef\nmv@citex@sfac3000\relax
\frenchspacing
    \mathchardef\nmv@citex@sfac1001\relax
1520
    \sfcode'\.\nmv@citex@sfac
1521
    \sfcode'\?\nmv@citex@sfac
1522
   \sfcode'\!\nmv@citex@sfac
1524 }
1525 \ifnum\sfcode'\.=\@m
1526 \frenchspacing
```

\nmv@citex@nat The swap has to be done at the beginning of the document. The internal flag \nmv@activate from natbib is used, but under the circumstances we should be safe. \cite is \cite also patched to make the system active.

```
1528 \newcommand*\nmv@citex@nat{}
1529 \newcommand*\nmv@activate{%
1530 \let\nmv@citex@nat\@citex
     \let\@citex\nmv@citex
     \let\nmv@cite\cite
1532
     \renewcommand*{\cite}[2][]{%
1533
       \nmv@ifmtarg{##1}{%
1534
          \nmv@citetrue
1535
          \nmv@cite{##2}%
1536
1537
          \nmv@citefalse
1538
          \nmv@cite[##1]{##2}}%
1539
1540
     }%
1541 }
```

\nmv@natbib@detect

So that natbib options can be set without worrying about load order, natmove doesn't require natbib. So a test is needed to see if it is actually loaded. This is done as a macro so that the effect can be changed by achemso.

```
1542 \newcommand*\nmv@natbib@detect{%
     \@ifpackageloaded{natbib}{%
1543
       \ifNAT@super
1544
          \expandafter\nmv@activate
1545
        \fi
1546
     }{%
1547
       \PackageInfo{natmove}{%
1548
          The natbib package is not loaded.\MessageBreak
1549
          Loading natmove will do nothing
1550
1551
1552
     }%
1553 }
1554 \AtBeginDocument{\nmv@natbib@detect}
```

\natmovechars A user macro is needed for moving characters.

```
1555 \newcommand*\natmovechars{.,;:}
1556 (/natmove)
```

## The configuration files

The configuration files for different journals are not very complex. Keeping everything separate simply helps with maintenance.

```
1557 (*achre4)
1558 \ProvidesFile{achemso-achre4.cfg}
    [2018/09/15 v3.12 achemso configuration: Acc. Chem. Res.]
1560 \setkeys{acs}{biblabel = plain}
1561 \def\acs@type@list{article,suppinfo}
1562 \def\abstractname{Conspectus}
1563 (/achre4)
1564 (*aaembp)
1565 \ProvidesFile{achemso-aaembp.cfg}
```

```
1566 [2018/09/15 v3.12 achemso configuration: ACS Appl. Electron. Mater.]
1567 \def\acs@type@list{article,letter,suppinfo}
1568 \setkeys{acs}{keywords = true}
1569 (/aaembp)
1570 (*aaemcq)
1571 \ProvidesFile{achemso-aaemcq.cfg}
1572 [2018/09/15 v3.12 achemso configuration: ACS Appl. Energy Mater.]
1573 \def\acs@type@list{article,letter,suppinfo}
1574 \setkeys{acs}{keywords = true}
1575 (/aaemcq)
1576 (*aamick)
1577 \ProvidesFile{achemso-aamick.cfg}
1578 [2018/09/15 v3.12 achemso configuration: ACS Appl. Mater. Interfaces]
1579 \def\acs@type@list{article,letter,suppinfo}
1580 \setkeys{acs}{keywords = true}
1581 (/aamick)
1582 (*aanmf6)
1583 \ProvidesFile{achemso-aanmf6.cfg}
1584 [2018/09/15 v3.12 achemso configuration: ACS Appl. Nano Mater.]
1585 \def\acs@type@list{article,letter,suppinfo}
1586 \setkeys{acs}{keywords = true}
1587 (/aanmf6)
1588 (*aapmcd)
1589 \ProvidesFile{achemso-aapmcd.cfg}
1590 [2018/09/15 v3.12 achemso configuration: ACS Appl. Polym. Mater.]
1591 \def\acs@type@list{article,letter,suppinfo}
1592 \setkeys{acs}{keywords = true}
1593 (/aapmcd)
1594 (*abseba)
1595 \ProvidesFile{achemso-abseba.cfg}
1596 [2018/09/15 v3.12 achemso configuration: ACS Biomater. Sci. Eng.]
1597 \setkeys{acs}{keywords = true}
1598 \def\acs@type@list{article,review,suppinfo}
1599 (/abseba)
1600 (*accacs)
1601 \ProvidesFile{achemso-accacs.cfg}
1602 [2018/09/15 v3.12 achemso configuration: ACS Catal.]
1603 \setkeys{acs}{keywords = true}
1604 \def\acs@type@list{article,letter,perspective,review,viewpoints,suppinfo}
1605 \SectionNumbersOff
1606 (/accacs)
1607 (*acscii)
1608 \ProvidesFile{achemso-acscii.cfg}
1609 [2018/09/15 v3.12 achemso configuration: ACS Central Sci.]
1610 \def\acs@type@list{article,review,suppinfo}
1611 \setkeys{acs}{doi = true}
1612 \SectionNumbersOff
1613 (/acscii)
1614 (*acbcct)
1615 \ProvidesFile{achemso-acbcct.cfg}
1616 [2018/09/15 v3.12 achemso configuration: ACS Chem. Biol.]
1617 \setkeys{acs}{
1618 biblabel = fullstop,
1619 biochem = true,
```

```
= false
1620
    super
1621 }
1622 \def\acs@type@list{article,letter,review,suppinfo}
1623 \SectionNumbersOff
1624 (/acbcct)
1625 (*acncdm)
1626 \ProvidesFile{achemso-acncdm.cfg}
     [2018/09/15 v3.12 achemso configuration: ACS Chem. Neurosci.]
1628 \def\acs@type@list{article,review,letter,suppinfo,viewpoint}
1629 \setkeys{acs}{
1630 biblabel = fullstop,
1631 biochem = true,
1632 keywords = true,
             = false
1633 super
1634 }
1635 (/acncdm)
1636 (*acsccc)
1637 \ProvidesFile{achemso-acsccc.cfg}
1638 [2018/09/15 v3.12 achemso configuration: ACS Combinatorial Sci.]
1639 \def\acs@type@list{article,letter,review,perspective,account,note,suppinfo}
1640 \setkeys{acs}{keywords = true}
1641 \SectionNumbersOff
1642 (/acsccc)
<sub>1643</sub> (*aesccq)
1644 \ProvidesFile{achemso-aesccq.cfg}
1645 [2018/09/15 v3.12 achemso configuration: ACS Earth Space Chem.]
1646 \def\acs@type@list{article,suppinfo}
1647 \setkeys{acs}{keywords = true}
1648 (/aesccq)
1649 (*aelccp)
1650 \ProvidesFile{achemso-aelccp.cfg}
1651 [2018/09/15 v3.12 achemso configuration: ACS Energy Lett.]
1652 \def\acs@type@list{letter,prespective,review,viewpoint,focus}
1653 \SectionsOff
1654 (/aelccp)
1655 (*ascefj)
1656 \ProvidesFile{achemso-ascefj.cfg}
1657 [2018/09/15 v3.12 achemso configuration: ACS Infect. Dis.]
1658 \def\acs@type@list{article,letter,prespective,review,viewpoint,suppinfo}
1659 \setkeys{acs}{keywords = true}
1660 \SectionsOff
1661 (/ascefj)
1662 (*amlccd)
1663 \ProvidesFile{achemso-amlccd.cfg}
1664 [2018/09/15 v3.12 achemso configuration: ACS Macro Lett.]
1665 \def\acs@type@list{letter,suppinfo}
1666 \SectionsOff
1667 \setlength{\acs@tocentry@height}{8 cm}
1668 \setlength{\acs@tocentry@width}{4 cm}
1669 (/amlccd)
1670 (*amclct)
1671 \ProvidesFile{achemso-amclct.cfg}
1672 [2018/09/15 v3.12 achemso configuration: ACS Med. Chem. Lett.]
1673 \def\acs@type@list{article,letter,perspective,suppinfo}
```

```
1674 \SectionNumbersOff
_{1675}\left</amclct\right>
1676 % \changes{v3.8n}{2015/01/13}{\emph{ACS Nano} want abbreviations}
_{1677}\% \ \text{changes}\{v3.11\}\{2018/04/02\}\{\text{Change } \text{emph}\{\text{ACS Nano}\} \ \text{truncation}\}
1678 (*ancac3)
1679 \ProvidesFile{achemso-ancac3.cfg}
1680 [2018/09/15 v3.12 achemso configuration: ACS Nano]
1681 \setkeys{acs}{
1682 abbreviations = true,
1683 biblabel = fullstop,
1684 etalmode
                    = truncate,
_{1685} maxauthors = 20,
                    = true
1686 keywords
1687 }
1688 \def\acs@type@list{article,perspective,suppinfo}
1689 \mbox{ latin}[1]{\mbox{ +1}}
1690 \SectionNumbersOff
1691 (/ancac3)
1692 (*acsodf)
1693 \ProvidesFile{achemso-acsodf.cfg}
1694 [2018/09/15 v3.12 achemso configuration: ACS Omega.]
1695 \def\acs@type@list{article}
1696 (/acsodf)
1697 (*apchd5)
1698 \ProvidesFile{achemso-apchd5.cfg}
1699 [2018/09/15 v3.12 achemso configuration: ACS Photon.]
1700 \def\acs@type@list{article,letter,perspective,review,suppinfo}
1701 \setkeys{acs}{keywords = true}
1702 \ifx\acs@manuscript\acs@manuscript@letter
1703 \SectionNumbersOff
1704\fi
_{1705}\left</\mathsf{apchd5}\right>
_{1706} (*aidcbc)
1707 \ProvidesFile{achemso-aidcbc.cfg}
     [2018/09/15 v3.12 achemso configuration: ACS Sensors]
1709 \def\acs@type@list{article,letter,perspective,review,suppinfo}
1710 \setkeys{acs}{keywords = true}
1711 \SectionNumbersOff
1712 (/aidcbc)
1713 (*ascecg)
1714 \ProvidesFile{achemso-ascecg.cfg}
1715 [2018/09/15 v3.12 achemso configuration: ACS Sustainable Chem Eng.]
1716 \setkeys{acs}{
1717 biblabel = fullstop,
1718 keywords = true
1719 }
1720 \SectionNumbersOff
1721 \def\acs@type@list{article,feature,letter,perspective,review,suppinfo}
1722 (/ascecg)
1723 (*asbcd6)
1724 \ProvidesFile{achemso-asbcd6.cfg}
1725 [2018/09/15 v3.12 achemso configuration: ACS Synth. Biol.]
1726 \setkeys{acs}{
1727 abbreviations = true,
```

```
biblabel
                      = fullstop,
1728
                      = true,
     biochem
1729
                      = true,
     keywords
1730
                      = false
     super
1731
1732 }
1733 \def\acs@type@list{article,letter,note,tutorial,review,suppinfo}
<sub>1734</sub> (/asbcd6)
1735 (*ancham)
1736 \ProvidesFile{achemso-ancham.cfg}
      [2018/09/15 v3.12 achemso configuration: Anal. Chem.]
1738 \def\acs@type@list{article,note,suppinfo}
1739 \SectionNumbersOff
1740 (/ancham)
_{1741} \langle *bichaw \rangle
1742 \ProvidesFile{achemso-bichaw.cfg}
      [2018/09/15 v3.12 achemso configuration: Biochemistry]
1744 \setkeys{acs}{
     abbreviations = true,
1746
     biblabel
                     = brackets,
1747
     biochem
                      = true,
1748}
1749 \SectionNumbersOff
{\tt 1750 \backslash def \backslash acs@maketitle@extras@hook{\%}}
      \par
1751
1752
      \acs@title@short@print
1753 }
_{1754} \g@addto@macro{\maketitle}{\newpage}
```

\acs@author@fnsymbol Some changes to do with footnotes: symbols are different and symbol number one can only be used for the title.

```
1755 \def\acs@author@fnsymbol#1{%
     \ensuremath{%
1756
        \ifcase #1 *\or
1757
          \dagger\or
1758
            \ddagger\or
1759
               \S\or
1760
                 \parallel\or
1761
                   \perp\or
1762
                      \P \
1763
                        \|\or
1764
                          \bot\or
1765
                            \tor
1766
                              @\or
1767
                                 \triangle\or
1768
                                   \nabla\else
1769
                                     #1%
1770
        \fi
1771
     }%
1772
1773 }
_{1774} \def\@maketitle@title@hook{%}
     \ifnum\acs@footnote@cnt>\@ne
1776
      \else
        \global\acs@footnote@cnt\@ne
1777
     \fi
1778
```

```
1779 }
1780 (/bichaw)
1781 (*bcches)
1782 \ProvidesFile{achemso-bcches.cfg}
1783 [2018/09/15 v3.12 achemso configuration: Bioconjugate Chem.]
1784 \setkeys{acs}{
1785 biochem = true,
_{1786} super = false
1787 }
_{17}88 \setminus SectionNumbersOff
1789 (/bcches)
1790 (*bomaf6)
1791 \ProvidesFile{achemso-bomaf6.cfg}
[2018/09/15 v3.12 achemso configuration: Biomacromolecules]
1793 \def\acs@type@list{article,comment,communication,note,review,suppinfo}
1794 \SectionNumbersOff
1795 \AtEndOfClass{\SectionsOn}
1796 (/bomaf6)
1797 (*crtoec)
1798 \ProvidesFile{achemso-crtoec.cfg}
_{1799} [2018/09/15 v3.12 achemso configuration: Chem. Res. Toxicol.]
1800 \setkeys{acs}{
1801 abbreviations = true,
1802 biochem
                   = true,
1803
    keywords
                   = true
1804 }
1805 \def\acs@maketitle@extras@hook{%
     \acs@title@short@print
1807
1808 }
1809 \def\acs@type@list{%
1810 article, perspective, profile, review, suppinfo%
1811 }
1812 \SectionNumbersOff
1813 (/crtoec)
1814 (*chreay)
1815 \ProvidesFile{achemso-chreay.cfg}
1816 [2018/09/15 v3.12 achemso configuration: Chem. Rev.]
1817 \def\acs@type@default{review}
1818 \def\acs@type@list{review}
The references section is numbered in Chem. Rev.
1819 \def\bibsection{\acs@section{\refname}}
1820 (/chreay)
1821 (*cmatex)
1822 %
        \begin{macrocode}
1823 \ProvidesFile{achemso-cmatex.cfg}
1824 [2018/09/15 v3.12 achemso configuration: Chem. Mater.]
1825 \setkeys{acs}{keywords = true}
1826 \SectionNumbersOff
1828 \AbstractOff
1829 \SectionsOff
1830\fi
```

```
1831 (/cmatex)
1832 (*cgdefu)
1833 \ProvidesFile{achemso-cgdefu.cfg}
1834 [2018/09/15 v3.12 achemso configuration: Cryst. Growth Des.]
1835 \def\acs@type@list{%
1836 article, communication, perspective, suppinfo%
1837 }
1838 \SectionNumbersOff
1840 \SectionsOff
1841\fi
_{1842} \stlength{\acs@tocentry@height}{8.9 cm}
1843 \setlength{\acs@tocentry@width}{4.6 cm}
_{1844}\left</\mathsf{cgdefu}\right>
1845 (*enfuem)
1846 \ProvidesFile{achemso-enfuem.cfg}
    [2018/09/15 v3.12 achemso configuration: Energy Fuels]
1848 \def\acs@type@list{article,review,suppinfo}
1849 \SectionNumbersOff
1850 (/enfuem)
1851 (*esthag)
1852 \ProvidesFile{achemso-esthag.cfg}
1853 [2018/09/15 v3.12 achemso configuration: Environ. Sci. Technol.]
1854 \def\acs@type@list{article,suppinfo}
1855 \SectionNumbersOff
1856 (/esthag)
1857 (*estlcu)
1858 \ProvidesFile{achemso-estlcu.cfg}
1859 [2018/09/15 v3.12 achemso configuration: Environ. Sci. Technol. Lett.]
1860 \def\acs@type@list{letter,suppinfo}
1861 \SectionNumbersOff
1862 (/estlcu)
_{1863} \changes{v3.8m}{2014/11/24}{Fixes for \emph{Ind.\ Eng.\ Chem.\ Res.}\ style}
1864 (*iecred)
1865 \ProvidesFile{achemso-iecred.cfg}
1866 [2018/09/15 v3.12 achemso configuration: Ind. Eng. Chem. Res.]
1867 \setkeys{acs}{biblabel = brackets}
1868 \SectionNumbersOff
1869 (/iecred)
1870 (*inoraj)
1871 \ProvidesFile{achemso-inoraj.cfg}
1872 [2018/09/15 v3.12 achemso configuration: Inorg. Chem.]
1873 \SectionNumbersOff
{\tt 1874 \setminus ifx \land acs@manuscript \land acs@manuscript@communication}
1875 \AbstractOff
    \SectionsOff
1876
1877 \fi
1878 \setkeys{acs}{doi = true}
1879 (/inoraj)
1880 (*jafcau)
1881 \ProvidesFile{achemso-jafcau.cfg}
1882 [2018/09/15 v3.12 achemso configuration: J. Agric. Food Chem.]
1883 \setkeys{acs}{keywords = true}
1884 \def\acs@type@list{article,suppinfo}
```

```
1885 \SectionNumbersOff
1886 (/jafcau)
1887 (*jceda8)
1888 \ProvidesFile{achemso-jceda8.cfg}
1889 [2018/09/15 v3.12 achemso configuration: J. Chem. Ed.]
1890 \setkeys{acs}{keywords = true}
1891 \SectionNumbersOff
1892 \def\acs@type@list{article,suppinfo}
1893 \SectionNumbersOff
1894 (/jceda8)
1895 (*jceaax)
1896 \ProvidesFile{achemso-jceaax.cfg}
    [2018/09/15 v3.12 achemso configuration: J. Chem. Eng. Data]
1898 \def\acs@type@list{article,suppinfo}
1899 \def\refname{Literature Cited}
1900 \SectionNumbersOff
1901 (/jceaax)
1902 (*jcisd8)
{\tt 1903 \ \ \ ProvidesFile\{achemso-jcisd8.cfg\}}
1904 [2018/09/15 v3.12 achemso configuration: J. Chem. Inf. Model.]
1905 \def\acs@type@list{article,suppinfo}
1906 \SectionNumbersOff
1907 (/jcisd8)
1908 (*jctcce)
1909 \ProvidesFile{achemso-jctcce.cfg}
1910 [2018/09/15 v3.12 achemso configuration: J. Chem. Theory Comput.]
1911 \def\acs@type@list{article,suppinfo}
1912 \setkeys{acs}{maxauthors = 0}
1913 (/jctcce)
1914 (*jmcmar)
1915 \ProvidesFile{achemso-jmcmar.cfg}
1916 [2018/09/15 v3.12 achemso configuration: J. Med. Chem.]
1917 \def\acs@type@list{article,letter,perspective,suppinfo}
1918 \SectionNumbersOff
1919 \setlength{\acs@tocentry@height}{5.5cm}
1920 \setlength{\acs@tocentry@width}{21cm}
1921 (/jmcmar)
1922 (*jnprdf)
1923 \ProvidesFile{achemso-jnprdf.cfg}
1924 [2018/09/15 v3.12 achemso configuration: J. Nat. Prod.]
1925 \renewcommand*{\abstractname}{ABSTRACT}
1927 \renewcommand*{\suppinfoname}{ASSOCIATED CONTENT}
1928 \SectionNumbersOff
1929 \renewcommand*{\acs@abstract}{%
1930
     \quotation
     \textbf{\abstractname :}%
1931
1932 }
1933 \AbstractOn
1934 \ifx\acs@manuscript\acs@manuscript@communication
    \AbstractOff
1936
    \SectionsOff
1937 \fi
1938 \def\refname{REFERENCES}
```

```
1939 \captionsetup{
1940 labelfont = bf,
1941 labelsep = period
1942 }
_{1943}\left</jnprdf\right>
1944 (*joceah)
1945 \ProvidesFile{achemso-joceah.cfg}
1946 [2018/09/15 v3.12 achemso configuration: J. Org. Chem.]
1948 \AbstractOff
    \SectionsOff
1949
1950 \fi
1951 \floatstyle{plaintop}
1952 \restylefloat{scheme}
1953 \floatstyle{plain}
1954 \renewcommand*\acs@type@list{article,communication,note,perspective,review,suppinfo}
1955 (/joceah)
1956 (*jpcafh)
1957 \ProvidesFile{achemso-jpcafh.cfg}
1958 [2018/09/15 v3.12 achemso configuration: J. Phys. Chem. A]
1959 \def\acs@type@list{article,suppinfo}
1960 \setkeys{acs}{
1961
    etalmode
                  = truncate,
1962
     maxauthors
1963 }
1964 \SectionNumbersOff
1965 \captionsetup[table] {labelfont=bf,textfont=bf}
1966 \g@addto@macro{\maketitle}{\newpage}
1967 (/jpcafh)
1968 (*jpcbfk)
1969 \ProvidesFile{achemso-jpcbfk.cfg}
1970 [2018/09/15 v3.12 achemso configuration: J. Phys. Chem. B]
1971 \def\acs@type@list{article,suppinfo}
1972 \setkeys{acs}{
    etalmode
                  = truncate,
1973
1974
     maxauthors
                  = 10
1975 }
1976 \SectionNumbersOff
1977 \captionsetup[table]{labelfont=bf,textfont=bf}
1979 (/jpcbfk)
1980 (*jpccck)
1981 \ProvidesFile{achemso-jpccck.cfg}
1982 [2018/09/15 v3.12 achemso configuration: J. Phys. Chem. C]
1983 \def\acs@type@list{article,suppinfo}
1984 \setkeys{acs}{
1985 etalmode
                  = truncate,
    maxauthors = 10
1986
1987 }
1988 \SectionNumbersOff
1989 \captionsetup[table] {labelfont=bf,textfont=bf}
1990 \g@addto@macro{\maketitle}{\newpage}
```

```
1991 (/jpccck)
1992 (*jpclcd)
1993 \ProvidesFile{achemso-jpclcd.cfg}
1994 [2018/09/15 v3.12 achemso configuration: J. Phys. Chem. Lett.]
1995 \setkeys{acs}{
1996 etalmode = truncate,
1997 maxauthors = 10
1998}
1999 \def\acs@type@default{letter}
2000 \def\acs@type@list{letter}
2001 \SectionNumbersOff
2002 \captionsetup[table]{labelfont=bf,textfont=bf}
2003 \g@addto@macro{\maketitle}{\newpage}
2004 \renewcommand{\acs@tocentry@print}[1]{%
     \gdef\acs@tocentry@text{#1}%
2006 }
2007 \renewcommand*{\acs@abstract@extras}{%
2008 \begingroup
       \acs@tocentry@print@aux
2000
     \endgroup
2010
     \acs@keywords@print
2011
     \newpage
2014 \setlength\acs@tocentry@height{2in}
2015 \setlength\acs@tocentry@width{2in}
2016 (/jpclcd)
2017 (*jprobs)
2018 \ProvidesFile{achemso-jprobs.cfg}
2019 [2018/09/15 v3.12 achemso configuration: J. Proteome Res.]
2020 \setkeys{acs}{keywords = true}
2021 \def\acs@type@list{article,review,suppinfo}
2022 \SectionNumbersOff
2023 (/jprobs)
 The J. Am. Chem. Soc. configuration is rather more complicated as there is the
 need to construct a "galley-like" layout for communications.
2024 (*jacsat)
2025 \ProvidesFile{achemso-jacsat.cfg}
2026 [2018/09/15 v3.12 achemso configuration: J. Am. Chem. Soc.]
2027 \SectionNumbersOff
2028 \ifx\acs@manuscript\acs@manuscript@communication\else
2029 \expandafter\endinput
2030\fi
 Everything from here onward applies only to communications. Some adjust-
 ments are now made using the existing tools.
2031 \setkeys{acs}{
2032 email = true,
2033 layout = twocolumn
2034 }
2035 \SectionsOff
2036 \acs@layout@nine
```

abstract The abstract appears at the start of the document, with lines around it.s

```
2037 \renewenvironment{abstract}{%
                                                                                      2038 \hrule
                                                                                      2039 \vspace{2 mm}%
                                                                                     2040 \sffamily
                                                                                     2041 \noindent
                                                                                      2042 \emph{\textbf{Abstract:}}%
                                                                                     2043 }{%
                                                                                                                         \vspace{2 mm}%
                                                                                      2044
                                                                                                                           \hrule
                                                                                                                          \vspace{6 mm}%
                                                                                      2046
                                                                                      2047 }
                      \acksize To keep things logical, the size macros are given names related to their function.
      \affilsize Some of these are new, some are defined in the class.
\authorsize _{2048} \det \affilsize {\%}
     \label{lem:lemailsize} $$\operatorname{2049} $$ \operatorname{Csetfontsize}\left(\frac{3}{2}\right) = \frac{1}{2} \left(\frac{3}{2}\right) =
                    \capsize 2050 }
                    \refsize 2051 \det \acksize{\%}
            \text{titlesize}^{2053}
                                                                                     2054 \def\authorsize{%
                                                                                     2055 \@setfontsize\authorsize{10.5}{12.5}%
                                                                                     2056 }
                                                                                     2057 \newcommand*\capsize{%
                                                                                     2058 \@setfontsize\capsize\@viiipt\@ixpt
                                                                                      2059 }
                                                                                      2060 \def\emailsize{%
                                                                                     2061 \@setfontsize\emailsize\@viiipt{15}%
                                                                                     2062 }
                                                                                     2063 \newcommand*\refsize{%
                                                                                                                           \@setfontsize\refsize{7.5}{7.5}%
                                                                                     2064
                                                                                     2065 }
                                                                                     2066 \def\suppsize{%
                                                                                     2067 \@setfontsize\suppsize{8.5}{10.5}%
                                                                                     2069 \left\langle \right\rangle 
                                                                                     2070 \@setfontsize\titlesize\@xiipt{13}%
                                                                                     2071 }
                                                                                     _{2072} \left| \text{let} \right|
                                                                                     2073 \le 
     \emailfont A slight font change.
                                                                                     2074 \ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath{\ensuremath}\amb}\amb}\amb}}}}}}}}}
               \ps@plain The header styles are done the hard way, to keep down the number of packages
                      \ps@jacs loaded.
                                                                                     2075 \def\ps@plain{%
                                                                                      2076 \let\@mkboth\@gobbletwo
                                                                                                                         \let\@oddhead\@empty
                                                                                     2078 \def\@oddfoot{%
                                                                                                                                        \reset@font
                                                                                     2079
                                                                                                                                         \sffamily
                                                                                     2080
                                                                                     2081
                                                                                                                                         \textbf{\thepage}%
                                                                                     2082
                                                                                                                                         \hfil
```

```
\let\@evenhead\@empty
                           2084
                                 \let\@evenfoot\@oddfoot
                           2085
                          2086 }
                          2087 \ensuremath{\mbox{def\ps@acs}{\mathcal{m}}}
                                 \def\@oddfoot{%
                           2088
                                   \reset@font
                           2089
                                   \sffamily
                           2090
                                   \textbf{\thepage}%
                                   \hfil
                           2092
                                }%
                           2093
                                 \def\@evenfoot{%
                           2094
                                   \reset@font
                           2095
                                   \hfil
                           2096
                                   \sffamily
                           2097
                                   \textbf{\thepage}%
                           2098
                           2099
                                 \def\@oddhead{}%
                           2101
                                 \let\@evenhead\@oddhead
                           2102 }
                           2103 \pagestyle{acs}
   \acs@space@pre@title Length adjustments for the title.
 \verb|\acs@space@post@title|| $_{2104} \le length \\ acs@space@pre@title{16mm}| 
 \verb|\acs@space@post@author||_{2105} \verb|\setlength| acs@space@post@title{Omm}|
\acs@space@post@address 2106 \setlength\acs@space@post@author{Omm}
  \acs@space@post@email 2107\setlength\acs@space@post@address{0mm}
                           2108 \setlength\acs@space@post@email{-1mm}
                           {\tt 2109 \backslash setlength \backslash acs@maketitle@width\{152.4mm\}}
   \acs@contact@details Contact details are different here.
                           2110 \def\acs@contact@details{%
                           2111 Received \today; E-mail: \acs@email@list
                           2112 }
 \acs@maketitle@extras No keywords or abbreviations for J. Am. Chem. Soc..
                           2113 \let\acs@maketitle@extras\relax
                            Getting the floats correct is a difficult task "by hand"; using the caption package
                            makes this a lot easier.
                           2114 \floatstyle{plaintop}
                           2115 \restylefloat{scheme}
                           2116 \floatstyle{plain}
                           2117 \DeclareCaptionLabelSeparator{perquad}{.\quad}
                           2118 \captionsetup{
                          2119 singlelinecheck = off,
                                labelfont
                                                  = {bf,it,sf},
                          2120
                                textfont
                                                  = sf,
                          2121
                                labelsep
                                                   = perquad
                          2122
                          2123 }
                           2124 \captionsetup[figure] {textfont=rm}
              \acs@table A patch or \table.
                   \table
```

}%

2083

```
2125 \newcommand*\acs@table{}
2126 \let\acs@table\table
2127 \left\ \frac{1}{2} \right\
     \capsize
2128
     \acs@table
2129
2130 }
 The bibliography has to be adjusted.
2131 \AtBeginDocument{%
     \def\bibsection{%
2132
        \@startsection
2133
          {section}
2134
2135
          {1}
          {\z0}{\z0}{\z0}{\z.5mm}%
2136
          {\normalfont\acksize\bfseries}
2137
          {\hrule\nobreak\vspace{1.2mm}\noindent\refname}%
2138
2139
     }%
2140
     \let\bibfont\refsize
     \verb|\setlength{\bibhang}{0.61cm}||
2141
     \setlength{\bibsep}{0mm}%
2142
2143 }
2144 (/jacsat)
2145 (*langd5)
2146 \ProvidesFile{achemso-langd5.cfg}
2147 [2018/09/15 v3.12 achemso configuration: Langmuir]
2148 \def\acs@type@list{article,letter,suppinfo}
_{2149} \SectionNumbersOff
2150 (/langd5)
_{2151} \langle *mamobx \rangle
2152 \ProvidesFile{achemso-mamobx.cfg}
2153 [2018/09/15 v3.12 achemso configuration: Macromolecules]
2154 \SectionNumbersOff
2155 \setkeys{acs}{doi = true}
2156 (/mamobx)
2157 (*mpohbp)
2158 \ProvidesFile{achemso-mpohbp.cfg}
    [2018/09/15 v3.12 achemso configuration: Mol. Pharm.]
2160 \setkeys{acs}{keywords = true}
2161 \def\acs@type@list{article,suppinfo}
2162 \SectionNumbersOff
2163 (/mpohbp)
2164 (*nalefd)
2165 \ProvidesFile{achemso-nalefd.cfg}
     [2018/09/15 v3.12 achemso configuration: Nano Lett.]
2167 \setkeys{acs}{keywords = true}
2168 \def\acs@type@default{letter}
2169 \def\acs@type@list{letter}
2170 \SectionNumbersOff
_{2171} \langle / nalefd\rangle
2172 (*orlef7)
[2018/09/15 \text{ v3.12 achemso configuration: Org. Lett.}]
2175 \def\acs@type@default{communication}
2176 \def\acs@type@list{communication}
```

```
_{2177}\SectionNumbersOff
2178 \setkeys{acs}{layout = twocolumn}
2179 \RequirePackage{xcolor}
{\tt 2180 \backslash definecolor\{orglett\}\{RGB\}\{128,0,0\}}
2181 (/orlef7)
_{2182} \langle *oprdfk \rangle
{\tt 2183 \backslash ProvidesFile\{achemso-oprdfk.cfg\}}
2184 [2018/09/15 v3.12 achemso configuration: Org. Proc. Res. Dev.]
2185 \def\acs@type@list{article,highlight,review,suppinfo}
_{2186} \setminus SectionNumbersOff
_{2187}\left\langle /\mathsf{oprdfk}\right\rangle
_{2188} (*orgnd7)
{\tt 2189} \verb|\ProvidesFile{achemso-orgnd7.cfg}|
2190 [2018/09/15 v3.12 achemso configuration: Organometallics]
_{2191} \SectionNumbersOff
2192 (/orgnd7)
```