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.

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1 Introduction

Support for BibT_EX bibliography following the requirements of the American Chemical Society (ACS), along with a package to make these easy to have been

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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.

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

¹For example, when writing a thesis.

- natbib
- setspace
- xkeyval

These are normally present in the current major T_EX 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.

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 1. If an unknown journal is specified, the package will fall-back on the journal=jacsat option.

manuscript

The second option is the manuscript option. This specifies the type of paper in the manuscript. The values here are article, note, communication, review, letter and perspective. The valid values will depend on the value of journal. The manuscript option determines whether sections and an abstract are valid. The value suppinfo is also available for supporting information.

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}
```

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

Table 1: Values for journal option

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}
```

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 Sometown, USA}
```

\and \thanks

\title

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.

The \title macro is extended to accept an optional argument. This is

²This will usually be the university or company name.

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

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.

doi

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.

 $\begin{array}{c} \text{\tt etalmode} \\ \text{\tt maxauthors} \end{array}$

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 BIBTEX. 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. $^{\text{I}}$

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_EX style files

achemso is supplied with two style files, achemso.bst and biochem.bst. The direct use of these without the achemso package file is not recommended, but is possible. The style files can be loaded in the usual way, with a \bibliographystyle command. The natbib 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 $BibT_EX$ style files implement the bibliographic style specified by the ACS in *The ACS Style Guide*. ² 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 BIBT_EX 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 text² some more text.
Some text ending a sentence.²
```

This is deactivated for other citation types.

```
Some text \citeyear{Coghill2006}.\\
Some text \citeauthor{Coghill2006}.\\
Some text \citenum{Coghill2006}.
Some text 2006.
Some text Coghill and Garson.
Some text 2.
```

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^2, more text.^2
Some text \cite{Coghill2006},
more text \cite{Coghill2006}.
```

8 Implementation

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}
3 [2020-07-21 v3.13b 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.

```
<sub>7</sub> ⟨*package⟩
8 \ProvidesPackage{achemso}
9 [2020-07-21 v3.13b Support for ACS journals]
10 \@ifclassloaded{achemso}{%
  \PackageInfo{achemso}{%
      You have already loaded the 'achemso' class:\MessageBreak
12
      loading the package will abort%
13
   }%
14
   \endinput
15
16 }{%
   \PackageInfo{achemso}{%
17
      When writing a submission to an ACS journal, please\MessageBreak
18
      use the achemso document class%
19
20
21 }
```

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

```
22 \newcommand*\acs@warning{\PackageWarning{achemso}}
23 (/package)
```

8.3 Common code

\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
    \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}

\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]{%
35 \acs@ifundefined{acs@#1#2}{%
36 \acs@warning{Unknown option '#2' for key #1}%
37 }{%
38 \@nameuse{acs@#1#2}%
39 }%
40}
```

\ifacs@abbreviations \ifacs@articletitle \ifacs@biochem \ifacs@chaptertitle \ifacs@doi \ifacs@email \ifacs@hyperref \ifacs@keywords \ifacs@super These are all very trivial definitions: to avoid issues with older versions of xkeyval each definition is done directly.

```
_{4^{1}}\newif\ifacs@abbreviations
 42 \newif\ifacs@articletitle
43 \newif\ifacs@biochem
 44 \newif\ifacs@doi
 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}%
 52 }
 53 \define@key{acs}{articletitle}[true]{%
 _{54} \acs@keyval@bool{articletitle}{#1}%
 55 }
 56 \define@key{acs}{biochem}[true]{%
     \acs@keyval@bool{biochem}{#1}%
 57
 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}%
 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}%
 69
 70 }
 71 \define@key{acs}{keywords}[true]{%
     \acs@keyval@bool{keywords}{#1}%
 73 }
 _{74} \ensuremath{\mbox{\sc open}} [true] {\%}
     \acs@keyval@bool{super}{#1}%
 76 }
 77 \define@key{acs}{usetitle}[true]{%
```

```
\acs@keyval@bool{articletitle}{#1}%
                   <sub>79</sub> }
                 Trivial again: done without using xkeyval for the same reasons as before.
   \acs@journal
    \acs@layout
                   80 \newcommand*\acs@journal{jacsat}
\acs@manuscript
                   81 \newcommand*\acs@layout{traditional}
                   82 \mbox{ 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}{%
                       \def\acs@layout{#1}%
                   89 }
                   90 \define@key{acs}{manuscript}{%
                      \def\acs@manuscript{#1}%
                   92 }
                   93 \define@key{acs}{maxauthors}{%
                       95 }
                 The setup for the etalmode option is quite simple: just look for the appropriate
```

\ifacs@etal@truncate \acs@etal@firstonly \acs@etal@truncate The setup for the etalmode option is quite simple: just look for the appropriate macros.

```
96 \newif\ifacs@etal@truncate
97 \define@key{acs}{etalmode}{%
    \acs@ifundefined{acs@etal@#1}{%
       \acs@warning{%
99
         Unknown value '#1' for\MessageBreak etalmode option%
101
    ጉና%
102
       \@nameuse{acs@etal@#1}%
103
    ጉ%
104
105 }
106 \newcommand*\acs@etal@firstonly{\acs@etal@truncatefalse}
107 \newcommand*\acs@etal@truncate{\acs@etal@truncatetrue}
```

\acs@activate@biblabel

The biochemistry option is an alias for biochem. The biblabel option is a 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}%
109
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
    }{%
       \acs@activate@biblabel{\@nameuse{acs@biblabel@#1}}%
117
    }%
118
119 }
120 \newcommand*\acs@activate@biblabel{}
```

```
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)
      \acs@biblabel@brackets
                               The macros to implement the idea above for biblabels.
      \acs@biblabel@fullstop
                                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}{
                                     email = true,
                                     super = true
                                136 }
                                Loading some other packages depends on the options chosen, so they are pro-
                                137 \ProcessOptionsX*<acs>
\acs@manuscript@communication
                               For text comparisons.
      \acs@manuscript@letter
                                138 \newcommand*\acs@manuscript@communication{communication}
         \acs@manuscript@note
                                139 \newcommand*\acs@manuscript@letter{letter}
      \acs@manuscript@review
                                140 \newcommand*\acs@manuscript@note{note}
    \acs@manuscript@suppinfo
                                141 \newcommand*\acs@manuscript@review{review}
                                142 \newcommand*\acs@manuscript@suppinfo{suppinfo}
                               To avoid needing to load the notes2bib package, especially as the plan is to move
             \acs@niib@create
                      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
                  \thebibnote
                               already having been loaded. To allow the package and class to behave differently
                     \bibnote
                 \bibnotemark
                               these are actually applied later.
                 \bibnotetext
                                143 \newcommand*\acs@niib@create{%
               \printbibnotes
                                     \@namedef{ver@notes2bib.sty}{%
                                144
                                       2009/04/20 v1.6a Integrating notes into the bibliography (achemso
                                145
                                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}%

\cite{##1}%

158

159

121 (*class)

```
\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
                           168
                                     \acs@bibliography{acs-\jobname}%
                           169
                                  \fi
                                }%
                           170
                           171 }
  \acs@niib@after@text After the text.
                           172 \newcommand*\acs@niib@after@text{}
                          The \acs@niib@text macro is the outer part of the writing system. It does not
        \acs@niib@text
                          absorb the text of note, as without \varepsilon-TFX 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
                           178
                                  \expandafter\acs@niib@no@write
                           179
                           180 }
       \acs@niib@write
                          Writing verbatim without \varepsilon-T<sub>E</sub>X.
 \acs@niib@write@aux@i
                           181 \newcommand*\acs@niib@write[1]{%
\acs@niib@write@aux@ii
                                \begingroup
                           182
                                  \let\do\@makeother
                           183
                                  \dospecials
                           184
                                  \catcode'\{ 1\relax
                           185
                                  \catcode'\} 2\relax
                           186
                                  \acs@niib@write@aux@i{#1}%
                           187
                           188 }
                              \newcommand*\acs@niib@write@aux@i[1]{%
                                \long\def\@tempa##1{%
                                     \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
                                \@tempa
                           198
                           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
```

\DeclareRobustCommand*{\bibnotetext}[1][\thebibnote]{%

160

161

```
206
                           \@esphack
                           \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
                      224
                           \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
                                \ncite{##2}%
                      231
                                \bibnote{Ref.~\citenum{##2}, ##1}%
                      232
                             }%
                      233
                           }%
                      234
                      235 }
                      236 \newcommand*\acs@autonote{\%}
                           \let\nmv@cite\cite
                      237
                           \renewcommand*{\cite}[2][]{%
                      238
                              \nmv@ifmtarg{##1}{%
                      239
                                \nmv@cite{##2}%
                      240
                      241
                                \nocite{##2}%
                      242
                                \bibnote{Ref.~\citenum{##2}, ##1}%
                      243
                             }%
                      244
                           }%
                      245
                      246 }
     \acs@bib@file
                     Some information or creating the control file for BtbT<sub>E</sub>X is set up.
  \acs@bib@message
                      247 \newwrite\acs@bib@file
     \acs@bib@name
                      248 \newcommand*\acs@bib@message{%
                           This is an auxiliary file used by the 'achemso' bundle. ^{-}J\%
                           This file may safely be deleted. It will be recreated as required. ^^J
                      250
                      252 \newcommand*\acs@bib@name{acs-\jobname.bib}
```

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

\acs@bibliography \bibliography 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
260
      \immediate\write\acs@bib@file{\acs@bib@message}%
261
      \edef\@tempa##1##2{%
262
        \space\space##1\space = "##2",^^J%
263
264
 265
      \immediate\write\acs@bib@file{%
 266
       @Control\string{%
          {\tt achemso-control, \^{^{}}} {\tt J} {\tt \%}
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
          \Otempa{ctrl-doi\space\space\space\space\space\space
274
            \space\space\space\f
275
            \ifacs@doi yes\else no\fi
276
          }%
277
278
          \Otempa{ctrl-etal-number\space\space\space}{\acs@maxauthors}%
          \@tempa{ctrl-etal-firstonly}{%
279
            \ifacs@etal@truncate no\else yes\fi
280
          }%
281
        \string}^^J%
282
     }%
283
      \immediate\write\@auxout{%
284
        \string\citation\string{achemso-control\string}%
285
 286
 287
      \AtEndDocument{%
        \immediate\closeout\acs@bib@file\relax
288
     }%
289
290 }
The \bibliography macro is now patched so that everything works correctly.
291 \AtBeginDocument{%
     \let\acs@bibliography\bibliography
     \def\bibliography#1{%
293
        \acs@bibliography{acs-\jobname,#1}%
294
     }%
295
296 }
```

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 \langle \text{/package} \mid \text{class} \rangle
```

8.4 Late class-only code

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 \text{setkeys{acs}}
303 abbreviations = false,
304 articletitle = true,
305 biblabel = brackets,
               = false,
306 biochem
                 = false,
307 doi
_{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
    {hyperref}
328 \AtBeginDocument{\doublespacing}
```

\title \@title For the meta-data, the REVT_EX bundle provides a good model for the commands to give the author. \gdef is used here to avoid any odd grouping issues.

```
\acs@title@short
```

```
329 \renewcommand*{\title}[2][]{%
330 \gdef\acs@title@short{#1}%
331 \gdef\@title{#2}%
332 \ifx\acs@title@short\@empty
333 \global\let\acs@title@short\@title
334 \fi
335 }
336 \@onlypreamble\title
```

\acs@author@cnt
\acs@affil@cnt
\acs@affil@alt@cnt

achemso tracks the number authors, affiliations and alternative affiliations.

337 \newcount\acs@author@cnt

```
338 \newcount\acs@affil@cnt
339 \newcount\acs@affil@alt@cnt
```

\acs@footnote@cnt \acs@affil@marker@cnt Two counts for getting affiliation footnotes correct.

```
340 \newcount\acs@footnote@cnt
341 \newcount\acs@affil@marker@cnt
```

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 \def\author#1{%
            \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}%
       349
            \endgroup
       350
       351 }
       352 \@onlypreamble\author
\and Neither \and nor \thanks are used by the document class.
       353 \det \frac{%}{2}
           \acs@warning{%
       354
              \string\and\space not used by the achemso class: please see
       355
```

```
\thanks
```

```
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
361
       the\MessageBreak the package documentation for details%
362
    }%
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
366
       \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 {\int } \pi = 1 
373
           \expandafter\gdef\csname @affil@\@roman\acs@affil@cnt\endcsname
374
             {#2}%
375
         \else
376
           \expandafter\gdef\csname @affil@\@roman\acs@affil@cnt\endcsname
377
```

```
378 {#1}%
379 \fi
380 }%
381 \else
382 \acs@warning{Affiliation with no author}%
383 \fi
384 }
385 \@onlypreamble\affiliation
```

\acs@affil@ifdup \acs@affil@ifdup@aux A short test for two addresses being identical.

```
386 \newcommand*\acs@affil@ifdup[1]{%
387
                    \begingroup
388
                            \def\@tempa{#1}%
389
                            \@tempswafalse
                            \@tempcnta\z@\relax
390
                            \acs@affil@ifdup@aux
391
 392
                            \if@tempswa
                                    \aftergroup\@firstoftwo
 393
                            \else
394
                                     \aftergroup\@secondoftwo
395
396
                    \endgroup
397
398 }
399 \newcommand*\acs@affil@ifdup@aux{%
                    \advance\@tempcnta\@ne\relax
400
                    \verb|\expandafter| expandafter| def| expandafter| expandaf
 401
                            \expandafter\@tempb\expandafter\expandafter\expandafter
 402
                            {\tt \{\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
411 }
```

\acs@affil@swap \acs@affil@swap@aux 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
       \advance\acs@affil@cnt\@ne\relax
418
       \acs@affil@swap@aux
419
     \endgroup
420
421 }
422 \newcommand*\acs@affil@swap@aux{%
    \advance\@tempcntb\@ne\relax
423
    \expandafter\ifnum\csname @author@affil@\@roman\@tempcntb\endcsname
424
       = \acs@affil@cnt\relax
425
```

\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} \mbox{ } \mbox{\  \  \ } \mbox{\  \  } \mbox{\  \  } \mbox{\  \  } \mbox{\  \  } \mbox{\  \  } \mbox{\  \  } \mbox{\  \  } \mbox{\  \  } \mbox{\  \
             \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 \frac{1}{relax}
443
                                \expandafter\gdef\csname @affil@\@roman\acs@affil@cnt\endcsname
444
                                      {#2}%
445
446
                                \expandafter\gdef\csname @affil@\@roman\acs@affil@cnt\endcsname
447
448
                                      {#1}%
                         \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
461
                    \acs@warning{Affiliation with no author}%
462
              \fi
463
464 }
465 \newcommand*\acs@alsoaffil@find[1]{%
             \begingroup
                    \def\def\def\#1%
467
                    \@tempcnta\z@\relax
468
                    \@tempcntb\z@\relax
469
                    \acs@affil@ifdup@aux
470
              \expandafter\endgroup
471
              \expandafter\@tempcnta\the\@tempcnta\relax
472
473 }
```

\altaffiliation For the alternative affiliation, a second count is kept, and the affiliation is "at-

tached" 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
       \begingroup
476
         \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
485
             \endcsname{\the\acs@affil@alt@cnt}%
486
487
       \endgroup
488
    \else
       \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
    497
      \expandafter\acs@altaffil@ifdup@aux
498
    \fi
499
    \if@tempswa
500
      \expandafter\@firstoftwo
501
502
       \expandafter\@secondoftwo
503
504
505 }
506 \newcommand*\acs@altaffil@ifdup@aux{%
    \advance\@tempcnta\@ne\relax
507
    \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
514
         \expandafter\expandafter\expandafter\acs@altaffil@ifdup@aux
515
      \fi
516
    \fi
517
518 }
```

\email E-mail addresses are attached to authors as well.

```
\ifnum\acs@author@cnt>\z@\relax
                                                                     520
                                                                                       \expandafter\gdef\csname @email@\@roman\acs@author@cnt\endcsname
                                                                     521
                                                                                            {#1}%
                                                                     522
                                                                     523
                                                                                       \acs@warning{E-mail with no author}%
                                                                     524
                                                                                 \fi
                                                                     525
                                                                     526 }
                                                                     527 \@onlypreamble\email
                                                                   Fax and phone numbers are similar.
                                               \phone
                                                                     528 \newcommand*\fax[1]{%
                                                                     529
                                                                                 \ifnum\acs@author@cnt>\z@\relax
                                                                                       \expandafter\gdef\csname @fax@\@roman\acs@author@cnt\endcsname
                                                                     530
                                                                                            {#1}%
                                                                     531
                                                                                 \else
                                                                     532
                                                                     533
                                                                                       \acs@warning{Fax number with no author}%
                                                                     534
                                                                     535 }
                                                                     536 \@onlypreamble\fax
                                                                     _{537} \rightarrow [1] {\%}
                                                                                 \ifnum\acs@author@cnt>\z@\relax
                                                                     538
                                                                                       \expandafter\gdef\csname @phone@\@roman\acs@author@cnt\endcsname
                                                                     539
                                                                                            {#1}%
                                                                     540
                                                                                  \else
                                                                     541
                                                                                      \verb|\acs@warning{Phone number with no author}|| % \end{minipage} % \end{mi
                                                                     542
                                                                                 \fi
                                                                     543
                                                                     544 }
                                                                     _{545}\ \@onlypreamble\phone
                                                                  Some journals use these.
                          \abbreviations
                       \@abbreviations
                                                                     546 \newcommand*\abbreviations[1]{%
                                       \keywords
                                                                                 \gdef\@abbreviations{#1}%
                                    \@keywords
                                                                     548 }
                                                                     549 \newcommand*\@abbreviations{}
                                                                      550 \@onlypreamble\abbreviations
                                                                     551 \newcommand*\keywords[1]{%
                                                                                 \gdef\@keywords{#1}%
                                                                    552
                                                                     553 }
                                                                     554 \newcommand*\@keywords{}
                                                                     555 \@onlypreamble\keywords
                                                                   For printing the key simple meta-data.
\acs@abbreviations@print
            \acs@keywords@print
                                                                     556 \newcommand*\acs@abbreviations@print{%
     \acs@title@short@print
                                                                                 \ifx\@abbreviations\@empty\else
                                                                     557
                                                                                       \section*{Abbreviations}
                                                                     558
                                                                                      \@abbreviations
                                                                     559
                                                                     560
                                                                                       \par
                                                                                 \fi
                                                                     561
                                                                     562 }
                                                                     563 \newcommand*\acs@keywords@print{%
                                                                                 \ifx\@keywords\@empty\else
                                                                     564
                                                                                       \section*{Keywords}
                                                                     565
                                                                                       \@keywords
                                                                     566
```

519 \newcommand*\email[1]{%

```
\par
                           567
                                \fi
                           568
                           569 }
                           570 \newcommand*\acs@title@short@print{%
                                \section*{Running header}
                           571
                                \acs@title@short
                           572
                                \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}
\acs@space@post@address
                           577 \newlength\acs@space@post@title
                           578 \setlength\acs@space@post@title{1.5em}
 \acs@space@post@email
                           579 \newlength\acs@space@post@author
   \acs@maketitle@width
                           580 \setlength\acs@space@post@author{1em}
                           581 \newlength\acs@space@post@address
                           582 \setlength\acs@space@post@address{1em}
                           _{583} \ensuremath{\ensuremath{\mbox{0space@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.
            \authorsize
                           587 \newcommand*\affilsize{\normalsize}
             \emailsize
                           588 \newcommand*\authorsize{\large}
             \titlesize
                           589 \newcommand*\emailsize{\normalsize}
                           590 \newcommand*\titlesize{\LARGE}
            \authorfont Font settings for \@maketitle.
            \authorfont
                           591 \newcommand*\affilfont{\itshape}
             \emailfont
                           592 \newcommand*\authorfont{\sffamily}
             \titlefont
                           593 \newcommand*\emailfont{}
                           594 \newcommand*\titlefont{\bfseries\sffamily}
                \ps@acs A shortcut to make page styles.
                           595 \newcommand*{\ps@acs}{}
                           596 \let\ps@acs\ps@plain
                          With the changes outlined above in place, a new \@maketitle macro is needed.
            \@maketitle
                          This is partially a copy of the existing, but rather heavily modified.
 \@maketitle@title@hook
                           597 \def\@maketitle{%
                                \pagestyle{acs}%
                           598
                                \ifnum\acs@author@cnt<\z@\relax
                           599
                                  \acs@warning{No authors defined: At least one author is required}%
                           600
                           601
                           602
                                \newpage
                                \null
                           603
                           604
                                \vspace*{\acs@space@pre@title}%
                           605
                                \begin{center}
                           606
                                  \begin{minipage}{\acs@maketitle@width}
                                    \begin{center}
                           607
                                      {%
                           608
```

```
\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
                                         }%
                             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
                                             \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
                             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]{%
                             654
                                  \footnotemark
                                   \g@addto@macro\@thanks{\footnotetext{#1}}%
                             655
                             656 }
                             657 \newcommand\acs@title@footnote@check{%
                             658 \ifx\@thanks\@empty
```

\titlefont

609

```
659
                              \else
                                \begingroup
                         660
                                  \toks@=\expandafter{\@thanks}%
                         661
                                  \xdef\@thanks{%
                         662
                                     \begingroup
                         663
                                       \let\noexpand\@fnsymbol\noexpand\acs@author@fnsymbol
                         664
                                       \the\toks@
                         665
                                     \endgroup
                         666
                                  }%
                         667
                         668
                                \endgroup
                         669
                              \fi
                         670 }
 \acs@contact@details
                        A general contact details macro.
                         671 \newcommand*\acs@contact@details{%
                              { \sffamily E-mail: \acs@email@list }%
                         673
                              \acs@number@list
                         674 }
                        The \Othanks macro is used as a hook to generate the footnotes if needed.
                         675 \let\@thanks\@empty
                        Printing the author list needs to do several things. The appropriate separators
     \acs@author@list
                        between authors are created and the author names themselves are printed.
                         676 \newcommand*\acs@author@list{%
                              \@tempcnta\z@\relax
                              \ifnum\acs@author@cnt=\z@\relax\else
                         678
                                \expandafter\acs@author@list@main
                         679
                              \fi
                         680
                         681 }
                        The main control macro for producing the author list iterates over each author
\acs@author@footnotes
\acs@author@list@main
                        on the list. The result is stored as \acs@author@listing.
                         682 \newcommand*\acs@author@footnotes{}
                         683 \newcommand*\acs@author@list@main{%
                              \advance\@tempcnta\@ne\relax
                              \def\acs@author@footnotes{}%
                         685
                              \acs@author@list@and
                         686
                              \space
                         687
                              \@nameuse{@author@\@roman\@tempcnta}%
                         688
                              \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

\ifnum\@tempcnta<\acs@author@cnt\relax

\expandafter\acs@author@list@main

\acs@author@footnotes%

694

695 696

697

698

699 700 } \fi

\acs@author@list@and \acs@author@list@comma

Simple checks to add an "and" and a 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
710
         ,%
711
       \fi
712
     \fi
713
714 }
```

\acs@author@star \acs@author@star@aux A check for an e-mail for an author: if so, add a star.

```
715 \newcommand*\acs@author@star{%
    \acs@author@star@aux
717
718
719 }
_{720} \ensuremath{\mbox{\sc Qauthor Qstar Qaux}} \%
    \protected@edef\acs@author@footnotes{%
721
      \acs@author@fnsymbol{\z@}%
722
      \ifnum\acs@affil@cnt>\@ne\relax
723
        ,%
724
      \else
725
        \ifnum\acs@affil@alt@cnt>\z@\relax
726
727
        \fi
728
      \fi
729
```

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

}%

730 731 }

The main affiliation of the author is checked for, and assuming one is found the appropriate symbol is added to the list.

```
732 \newcommand*\acs@author@affil{%
    \acs@ifundefined{%
733
       @affil@\@roman\csname @author@affil@\@roman\@tempcnta\endcsname
734
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 \newcommand*\acs@author@affil@also{%
    765
766
       \acs@author@affil@also@aux
767
768 }
_{769} \mbox{\ensuremath{\mbox{\sc Qauthor Qaffil Qalso Qaux}}} \%
    \expandafter\@for\expandafter\@tempa\expandafter:\expandafter
      =\csname @author@alsoaffil@\@roman\@tempcnta\endcsname\do{%
771
      \verb|\acs@affil@marker@cnt@tempa| relax|
772
      \advance\acs@affil@marker@cnt\acs@footnote@cnt\relax
773
      \protected@edef\acs@author@footnotes{%
        \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@author@affil@alt@aux
783
    }%
784
785 }
786 \newcommand*\acs@author@affil@alt@aux{%
    \expandafter\acs@affil@marker@cnt
787
      \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 }
```

\acs@author@fnsymbol
acs@author@fnsymbol@loop
cs@author@fnsymbol@loop@aux@i
s@author@fnsymbol@loop@aux@i
cs@author@fnsymbol@loop@aux@m
cs@author@fnsymbol@loop@aux@Q
\acs@author@fnsymbol@loop@aux@Q

The ACS have an extended list of symbols. The star appears at the special position zero.

```
797 \newcommand*{\acs@author@fnsymbol}[1]{%
     \ensuremath{%
798
       \expandafter\acs@author@fnsymbol@aux\expandafter{\number#1 }%
799
800
801 }
802 \newcommand*{\acs@author@fnsymbol@aux}[1]{%
803
     \ifnum#1>10 %
804
       \expandafter\acs@author@fnsymbol@loop
805
     \else
       \expandafter\acs@author@fnsymbol@symbol
806
     \fi
807
       {#1}%
808
809 }
810 \newcommand*{\acs@author@fnsymbol@loop}[1]{%
      \acs@author@fnsymbol@loop@aux@i#1%
811
812 }
813 \mbox{ newcommand} {\acs@author@fnsymbol@loop@aux@i}[2]{%}
     \acs@author@fnsymbol@symbol{\ifnum#2=0 10\else #2\fi}\%
     \expandafter\acs@author@fnsymbol@loop@aux@ii\romannumeral #1000Q{}%
815
816
       {\acs@author@fnsymbol@symbol{\ifnum#2=0 10\leq #2\fi}}%
817 }
818 \mbox{ newcommand} {\acs@author@fnsymbol@loop@aux@ii} [1] {% }
     \@nameuse{acs@author@fnsymbol@loop@aux@#1}%
819
820 }
821 \def\acs@author@fnsymbol@loop@aux@m#1Q#2#3{%
     \acs@author@fnsymbol@loop@aux@ii#1Q{#2#3}{#3}%
822
823 }
824 \mbox{\newcommand} {\acs@author@fnsymbol@loop@aux@Q}[2]{#1}
825 \newcommand*{\acs@author@fnsymbol@symbol}[1]{%
     \ifcase #1 *\or
826
       \dagger\or
827
         \ddagger\or
828
            \P\or
829
              \S\or
830
                \|\or
831
                  \bot\or
832
                    \#\or
833
834
                         \triangle\or
835
                           \nabla
836
       \fi
837
838 }
```

\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{%
840 \ifnum\acs@affil@cnt>\z@
841 \expandafter\acs@address@list@auxi
842 \else
843 \acs@warning{No affiliations: at least one affiliation is needed}%
844 \fi
```

```
845 }
846 \newcommand*\acs@address@list@auxi{%
     \ifnum0%
847
       \ifnum\acs@affil@cnt>\@ne
                                      1\fi
848
       \ifnum\acs@affil@alt@cnt>\z@ 1\fi
849
850
       \expandafter\acs@address@list@auxii
851
852
853
       \@address@i\par
     \fi
854
855 }
856 \newcommand*\acs@address@list@auxii{%
     \@tempcnta\z@
857
     \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}%
       \@nameuse{@address@\@roman\@tempcnta}\par
863
     \repeat
864
     \@tempcnta\z@
865
     \loop\ifnum\@tempcnta<\acs@affil@cnt
866
       \advance\@tempcnta\@ne
867
       \advance\acs@affil@marker@cnt\@ne
868
869
       \acs@ifundefined{@altaffil@\@roman\@tempcnta}
         {}
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{%
    \let\acs@fnsymbol@org\@fnsymbol
879
    \let\@fnsymbol\acs@author@fnsymbol
880
    \@tempcnta\z@\relax
881
     \@tempcntb\z@\relax
882
     \ifnum\acs@affil@cnt>\@ne\relax
883
884
       \expandafter\acs@affil@list@aux
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
891
892
     \ifnum\acs@affil@alt@cnt>\z@\relax
893
       \expandafter\acs@affil@alt@list
```

```
\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
900
     \advance\acs@affil@marker@cnt\acs@footnote@cnt\relax
901
     \footnotetext[\acs@affil@marker@cnt]{%
902
       \@nameuse{@affil@\@roman\@tempcnta}%
903
904
     \ifnum\@tempcnta<\acs@affil@cnt\relax
       \expandafter\acs@affil@list@aux
906
     \fi
907
908 }
```

\acs@affil@alt@list \acs@affil@alt@lista@aux The secondary loop for alternative affiliations is similar.

```
909 \newcommand*\acs@affil@alt@list{%
     \advance\@tempcntb\@ne\relax
910
     \acs@ifundefined{@altaffil@\@roman\@tempcntb}{}{%
911
       \acs@altaffil@foot@aux
912
913
     \ifnum\@tempcntb<\acs@author@cnt\relax
914
       \expandafter\acs@affil@alt@list
915
916
     \fi
917 }
918 \mbox{ \newcommand*\acs@altaffil@foot@aux{\%}}
     \advance\@tempcnta\@ne\relax
919
     \acs@affil@marker@cnt\@tempcnta\relax
920
     \advance\acs@affil@marker@cnt\acs@footnote@cnt\relax
921
     \footnotetext[\acs@affil@marker@cnt]{%
922
       \@nameuse{@altaffil@\@roman\@tempcntb}%
923
     }%
924
925 }
```

\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 \newcommand*\acs@email@list@aux{%
```

```
\advance\@tempcnta\@ne\relax
     \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
           \protected@edef\@tempa{%
966
             \@tempb.\space\@tempa
967
968
         \fi
969
       \fi
970
       \ifx\@tempa\@empty\else
971
         \par
972
         \@tempa
973
       \fi
974
     \endgroup
975
976 }
977 \newcommand*\acs@number@list@aux@i[1]{%
    \def\@tempa{}%
978
     \@tempcnta\z@\relax
979
     \def\acs@number@list@aux@ii{%
980
981
       \advance\@tempcnta\@ne\relax
      \ifnum\@tempcnta>\acs@author@cnt\relax\else
982
         983
           \acs@ifundefined{@email@\@roman\@tempcnta}{}{%
984
             \ifx\@tempa\@empty
985
               \edef\@tempa{%
986
                 \@nameuse{@#1@\@roman\@tempcnta}%
987
               }%
988
             \else
989
               \edef\@tempa{%
990
                 \@tempa
991
```

```
\@nameuse{@#1@\@roman\@tempcnta}%
                               993
                                               }%
                               994
                                             \fi
                               995
                                          }%
                               996
                                        }%
                               997
                                        \expandafter\acs@number@list@aux@ii
                               998
                               999
                                    }%
                              1000
                                    \acs@number@list@aux@ii
                              1001
                                    \ifx\@tempa\@empty\else
                              1002
                                      \protected@edef\@tempa{%
                              1003
                                         \MakeUppercase#1: \@tempa
                              1004
                                      }%
                              1005
                                    \fi
                              1006
                              1007 }
                              1008 \newcommand*\acs@number@list@aux@ii{}
               \endabstract
      \acs@abstract@extras
                              1009 \g@addto@macro\endabstract{%
                                    \aftergroup\acs@abstract@extras
                              1010
                              1011 }
                              1012 \newcommand*{\acs@abstract@extras}{%
                                    \ifacs@abbreviations
                              1013
                                      \acs@abbreviations@print
                              1014
                                      \par
                              1015
                                    \fi
                              1016
                                    \ifacs@keywords
                              1017
                                      \acs@keywords@print
                              1018
                                      \par
                              1019
                                    \fi
                              1020
                              1021 }
                              A couple of things might need to be added to \maketitle.
     \acs@maketitle@extras
\acs@maketitle@extras@hook
                              1022 \newcommand*\acs@maketitle@extras{%
                                    \acs@maketitle@extras@hook
                              1023
                              1024 }
                              1025 \newcommand*\acs@maketitle@extras@hook{}
                              1026 \g@addto@macro{\maketitle}{\acs@maketitle@extras}
                              \maketitle is required by the document class, and must start the document. No
                              variation is allowed, and so it is done automatically.
                              1027 \g@addto@macro{\document}{\maketitle}
                              Three new float types are provided, scheme, chart and graph. These are the
                     scheme
                              most obvious types; for graphs, a slight problem arises with the file extension.
                      chart
                      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}
```

992

```
\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}
                                                Both the numbering and existence of section headers may need to be altered.
                    \acs@section
                                                 Some generic functions are therefore provided to deal with this cleanly. First,
              \acs@subsection
        \acs@subsubsection
                                                 some original definitions are saved.
\acs@startsection@orig
                                                 1048 \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
                                                  1059 \@afterindenttrue
                                                  1060 \ifdim \@tempskipa <\z@ \@tempskipa -\@tempskipa \@afterindentfalse\fi
                                                  1061 \if@nobreak \everypar{}\else
                                                                   \addpenalty\@secpenalty\addvspace\@tempskipa\fi
                                                  1062
                                                  1063 \@ifstar{\@dblarg{\@sect{#1}{\@m}{#3}{#4}{#5}{#6}}}%
                                                                           {\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\d}_{\d}^{\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
                                                  1065 }
                                                  1066 \let\@startsection\acs@startsection
 \acs@startsection@alt An alternative version of \@startsection which never adds numbers.
                                                 1067 \newcommand*\acs@startsection@alt[6]{%
                                                  1068 \if@noskipsec \leavevmode \fi
                                                            \par \@tempskipa #4\relax
                                                  1060
                                                  1070 \@afterindenttrue
```

```
\if@nobreak \everypar{}\else
                                  \addpenalty\@secpenalty\addvspace\@tempskipa\fi
                         1073
                              \@ifstar{\@ssect{#3}{#4}{#5}{#6}}
                         1074
                                       {\@ssect{#3}{#4}{#5}{#6}}%
                         1075
                         1076 }
                         When removing sections entirely, a gobble macro is needed.
    \acs@sections@none
\acs@sections@none@aux
                         1077 \newcommand*\acs@sections@none{%
                              \@ifstar{%
                         1078
                                \acs@sections@none@aux
                         1079
                         1080
                         1081
                                 \acs@sections@none@aux
                         1082
                         1083 }
                         1084 \newcommand*\acs@sections@none@aux[2][]{%
                         1085
                              \acs@warning{%
                         1086
                                 (Sub)section '#2' ignored%
                         1087
                              }%
                         1088 }
                        To macros to add or remove the section numbers. The standard setting for the
    \SectionNumbersOff
     \SectionNumbersOn
                        class has them on, but some configurations will turn them off. The names of
                         these functions are both in design space so that users can change the decision
                         1089 \newcommand*\SectionNumbersOff{%
                              \let\@startsection\acs@startsection@alt
                         1090
                         1091 }
                         1092 \@onlypreamble\SectionNumbersOff
                         1093 \newcommand*\SectionNumbersOn{%
                              \let\@startsection\acs@startsection
                         1095 }
                         1096 \@onlypreamble\SectionNumbersOn
                        Quite similar for entire sections.
          \SectionsOff
           \SectionsOn
                         1097 \newcommand*\SectionsOff{%
                              \let\section\acs@sections@none
                              \let\subsection\acs@sections@none
                         1099
                              \let\subsubsection\acs@sections@none
                         1100
                         1101 }
                         1102 \@onlypreamble\SectionsOff
                         1103 \newcommand*\SectionsOn{%
                              \let\section\acs@section
                              \let\subsubsection\acs@subsubsection
                         1106
                         1107 }
                         1108 \@onlypreamble\SectionsOn
                        Never print TOC in itself.
      \tableofcontents
                         1109 \begingroup
                              \toks@=\expandafter{\tableofcontents}
                              \xdef\tableofcontents{%
                         1111
                                \begingroup
                         1112
```

```
\let\noexpand\@startsection\noexpand\acs@startsection@orig
                        1113
                                  \the\toks@
                        1114
                                \endgroup
                        1115
                             }
                        1116
                        1117 \endgroup
                        Simple named sections.
      acknowledgement
             suppinfo
                        1118 \newenvironment{acknowledgement}{%
                        1119 \acs@section*{\acknowledgementname}%
                        1120 }{}
                        1121 \newenvironment{suppinfo}{%
                             \acs@section*{\suppinfoname}%
 \acknowledgementname
                        A few macros need to get around the changes.
          \bibsection
                        1124 \newcommand*\acknowledgementname{Acknowledgement}
        \suppinfoname
                        1125 \AtEndOfClass{%
                              \def\bibsection{%
                                \acs@section*{\refname}%
                        1128
                        1129 }
                        1130 \newcommand*\suppinfoname{Supporting Information Available}
                        Removing the abstract, if necessary, is done using a trick from the comment
        \acs@abstract
     \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
                             \catcode'{ \active
                        1136
                              \catcode'} 12\relax
                        1137
                              \catcode'( 1\relax
                        1138
                              \catcode') 2\relax
                        1139
                              \gdef\acs@abstract@start(%
                        1140
                                \acs@warning(%
                        1141
                                  Abstract not allowed for this\MessageBreak
                        1142
                                   manuscript type
                        1143
                                )%
                        1144
                                \@bsphack
                        1145
                                \catcode'{ \active
                        1146
                                \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
```

```
1160
                               \else
                                  \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{%
                             \let\abstract\acs@abstract@start
                             \let\endabstract\acs@abstract@end
                       1169 }
                       1170 \@onlypreamble\AbstractOff
                       1171 \newcommand*\AbstractOn{%
                            \let\abstract\acs@abstract
                             \let\endabstract\acs@endabstract
                       1174 }
                       1175 \@onlypreamble\AbstractOn
   \acs@collect@toks
                       The content of the graphic TOC entry is processed using a method from amsmath
                       via environ. The entire environment is gathered for typesetting in a box. First,
\acs@collect@content
\acs@collect@content
                       some storage is needed.
                       1176 \newtoks\acs@collect@toks
                       1177 \newtoks\acs@collect@empty@toks
                       1178 \newcommand*\acs@collect@begins{}
                       1179 \newcommand*\acs@collect@content{}
                       This is a \long version of \collect@body.
        \acs@collect
    \acs@collect@aux
                       1180 \newcommand\acs@collect[1]{%
\acs@collect@begins@
                             \acs@collect@toks{%
                       1181
                               \expandafter#1\expandafter{\the\acs@collect@toks}%
   \acs@collect@body
                       1182
                       1183
                             \edef\acs@collect@content{%
                       1184
                               \the\acs@collect@toks
                       1185
                               \noexpand\end{\@currenvir}%
                       1186
                       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
                               \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{%
                       1199
                               \verb|\acs@collect@begins@#1\begin\end|
                       1200
                               \expandafter\@gobble\acs@collect@begins
                       1201
                       1202
                             \ifx\@empty\acs@collect@begins
                       1203
                               \endgroup
                       1204
                               \@checkend{#2}%
                       1205
```

```
\acs@collect@body{#1}%
1206
      \else
1207
        \acs@collect@body{\#1\end{\#2}}\%
1208
      \fi
1209
      \acs@collect@content
1210
1211 }
1212 \newcommand*\acs@collect@begins@{}
1213 \long\def\acs@collect@begins@#1\begin#2{%
      \fx\end#2\else
        b\expandafter\acs@collect@begins@
1215
1216
1217 }
1218 \newcommand\acs@collect@body[1]{%
      \global\acs@collect@toks\expandafter{\the\acs@collect@toks#1}%
1219
1220 }
```

\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
        \else
1225
          \@restonecolfalse\newpage
1226
1227
        \acs@section*{Abstract}%
1228
        #1%
1229
        \if@restonecol
1230
          \twocolumn
1231
        \else
1232
          \newpage
1233
        \fi
1234
     }%
1235
      \AtEndDocument{\acs@abstract@text}%
1236
1237 }
```

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

```
1238 \newcommand{\acs@tocentry@print}[1]{%
      \gdef\acs@tocentry@text{\normalsize#1}%
1239
      \AtEndDocument{%
1240
        \if@twocolumn
1241
          \@restonecoltrue\onecolumn
1242
1243
          \@restonecolfalse\newpage
1244
1245
        \acs@tocentry@print@aux
1246
        \if@restonecol
1247
1248
          \twocolumn
        \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
                            \tocsize
                    1258
                            \sffamily
                    1259
                            \singlespacing
                    1260
                            \begin{center}
                    1261
                    1262
                              \fbox
                    1263
                                ፈ%
                                   \begin{minipage}{\acs@tocentry@width}
                    1264
                                     \vbox to \acs@tocentry@height{\acs@tocentry@text}%
                    1265
                                   \end{minipage}%
                    1266
                                }%
                    1267
                            \end{center}%
                    1268
                          \endgroup
                    1269
                    1270 }
                    1271 \newcommand*\acs@tocentry@text{TOC ENTRY REQUIRED}
                    1272 \newlength{\acs@tocentry@height}
                    1273 \newlength{\acs@tocentry@width}
                    1274 \setlength{\acs@tocentry@height}{1.75in}
                    1275 \setlength{\acs@tocentry@width}{3.25in}
         tocentry Actually creating the entry is pretty easy.
                    1276 \newenvironment{tocentry}{\acs@collect\acs@tocentry@print}{}
    \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
                    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{%
                          \@tempswafalse
                    1284
                          \@for\@tempa:=\acs@type@list\do{%
                    1285
                            \ifx\@tempa\acs@manuscript
                    1286
                    1287
                              \expandafter\@tempswatrue
                    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
                    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}%
                     1303
                           \def\acs@type@list{#2}%
                     1304 }
          \acs@par A saved paragraph.
                     1305 \newcommand*\acs@par{}
                     1306 \let\acs@par\par
                     Some code is used generally when setting up "press ready" layouts. There is
\acs@layout@shared
                     quite a bit here, mainly layout related.
   acknowledgement
          suppinfo
                     1307 \newcommand*\acs@layout@shared{%
                           \AtBeginDocument{\singlespacing}%
                           \twocolumn
                     1309
                           \tolerance=2000\relax
                           \emergencystretch=10pt\relax
                     1311
                           \geometry{
                     1312
                             letterpaper,
                     1313
                             top = 12.7mm,
                     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
                               \vspace{6pt}%
                     1326
                               \textbf{\acknowledgementname}%
                     1327
                     1328
                               \acs@section*{\acknowledgementname}%
                     1329
                             \fi
                     1330
                           }{%
                     1331
                             \acs@par
                     1332
                           }%
                     1333
                     1334 }
                     More sizes.
          \acksize
         \suppsize
                     1335 \newcommand*\acksize{\normalsize}
                     1336 \newcommand*\suppsize{\normalsize}
                     The class loads twelve point text. To reset it for print layouts, it is easiest to do
  \acs@layout@nine
                     things directly.
             \@xipt
   \acs@layout@ten
                     1337 \newcommand*\acs@layout@nine{%
                           \def\@xipt{11}%
                     1338
                           \long\def\normalsize{%
```

1339

```
}%
          1341
                \normalsize
          1342
                \let\@listi\@listI
          1343
                \abovedisplayskip 5\p@ \@plus2\p@ \@minus 5\p@\relax
          1344
                \abovedisplayshortskip \z@ \@plus3\p@\relax
          1345
                \belowdisplayshortskip 3\p@ \@plus3\p@ \@minus 3\p@\relax
          1346
                \belowdisplayskip\abovedisplayskip\relax
          1347
                \abovecaptionskip 5\p@\relax
          1348
                \intextsep 7\p@ \@plus 2\p@ \@minus 2\p@\relax
          1349
          1350 }
          1351 \newcommand*\acs@layout@ten{%
                \long\def\normalsize{%
          1352
                  \@setfontsize\normalsize\@xpt\@xiipt
          1353
          1354
                \normalsize
          1355
                \@setfontsize\normalsize\@xpt\@xiipt
          1356
                \let\@listi\@listI
          1357
                \abovedisplayskip 10\p@ \@plus2\p@ \@minus5\p@\relax
          1358
                \abovedisplayshortskip \z@ \@plus3\p@\relax
                \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{%
                  Unknown journal '\acs@journal':\MessageBreak
          1365
                  using default configuration JACSAT%
          1366
          1367
                \input{achemso-jacsat.cfg}%
          1368
          1369 }
          Some changes that can always be applied if the manuscript type is appropriate:
\thepage
          this saves some repetition in the configuration files.
          1370 \acs@type@check
          1371 \ifx\acs@manuscript\acs@manuscript@note
          1372 \SectionsOff
          1373 \fi
          1374 \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}
          1382
                \renewcommand*\thetable{S\@arabic\c@table}
          1383
                \AtBeginDocument
          1384
                  ₹%
          1385
                    \renewcommand*\citenumfont[1]{S#1}%
          1386
                    \renewcommand*\bibnumfmt[1]{(S#1)}%
          1387
          1388
```

\@setfontsize\normalsize\@ixpt\@xipt

1340

```
1389\fi
```

Set up two column layout.

```
1390 \begingroup
     \def\@tempa{twocolumn}
      \ifx\acs@layout\@tempa
1392
        \aftergroup\acs@layout@shared
1393
1394
      \def\@tempa{two-column}
1395
     \ifx\acs@layout\@tempa
1396
        \aftergroup\acs@layout@shared
1397
1398
1399 \endgroup
1400 (/class)
```

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
     \RequirePackage[sort&compress,numbers,super]{natbib}
1403
1404 \else
     \RequirePackage[sort&compress,numbers,round] {natbib}
     \def\citenumfont{\textit}
1406
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
      \else
1414
        \setcitestyle{round}%
1415
        \renewcommand*\citenumfont{\textit}
1416
     \fi
1417
1418 }
1419 \RequirePackage{natmove}
```

The mciteplus package allows the construction of lists of references with sub-letters. 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 cross-references 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}{%
1421 \RequirePackage{mciteplus}
1422 \providecommand*{\@mciteNatbibCiteCmdList}{}%
1423 \edef\@tempa{\noexpand\in@{citenum}{\@mciteNatbibCiteCmdList}}%
1424 \@tempa
1425 \iffin@
1426 \else
```

```
% large lar
```

\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
1435 \def\acs@bibstyle{biochem}
1436 \bibliographystyle{biochem}
1437 \else
1438 \bibliographystyle{achemso}
1439 \fi
```

\acs@bibliographystyle \bibliographystyle

The original \bibliographystyle macro is now disabled: the underlying command is repeated otherwise problems cop up with chapterbib.

```
1440 \newcommand*\acs@bibliographystyle{}
1441 \let\acs@bibliographystyle\bibliographystyle
1442 \def\bibliographystyle#1{%
1443 \acs@warning{\string\bibliographystyle\space ignored}%
1444 \expandafter\acs@bibliographystyle\expandafter{\acs@bibstyle}%
1445 }
1446 \class | package\
```

8.6 Late package-only code

The notes2bib code may or may not be activated.

```
1447 (*package)
1448 \AtBeginDocument{%
1449 \@ifpackageloaded{notes2bib}{}{%
1450 \acs@niib@create
1451 }%
1452 }
1453 (/package)
```

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.

```
\begin{array}{l} _{1454} \left<^* natmove\right> \\ _{1455} \left<^* natmove\right> \\ _{1456} \left[ 2010/01/15 \ v1.1a \ Automatic \ citation \ moving \ with \ natbib \right] \\ _{1457} \left<^* RequirePackage\{natbib\} \right. \end{array}
```

\nmv@ifmtarg \nmv@xifmtarg

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

```
1458 \newcommand*\nmv@ifmtarg{}
1459 \newcommand*\nmv@xifmtarg{}
```

```
1460 \begingroup
                                   \catcode'\Q 3\relax
                             1461
                                   \long\gdef\nmv@ifmtarg#1{%
                             1462
                                      \nmv@xifmtarg#1QQ\@secondoftwo\@firstoftwo\@nil
                             1463
                             1464
                                   \label{longdefnmv0xifmtarg#1#2Q#3#4#5\0ni1{#4}} $$ \label{longdefnmv0xifmtarg#1#2Q#3#4#5\0ni1{#4}} $$
                             1465
                             1466 \endgroup
                            A flag is need to watch whether \cite or another macro is in use.
               \ifnmv@cite
                             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{%
                                   \ifnmv@cite
                             1469
                                      \expandafter\nmv@citex@moving
                             1470
                             1471
                                      \expandafter\nmv@citex@nat
                             1472
                             1473
                             1474 }
                \nmv@after Later, the argument for \cite will need to be saved.
                             1475 \newcommand*\nmv@after{}
                             The new version of \@citex is needed that looks ahead of the citation using
        \nmv@citex@moving
                             \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{%
                                   \leavevmode
                                   \skip@\lastskip\relax
                             1479
                             1480
                                   \unskip
                                   \begingroup
                             1481
                                      \def\nmv@after{\nmv@citex@nat[#1][#2]{#3}}%
                             1482
                                      \global\nmv@citefalse
                             1483
                                      \nmv@citex@get@next\relax
                             1484
                             1485 }
                             To get things right at the end.
            \nmv@citex@end
                             1486 \newcommand*\nmv@citex@end{%
                                      \nmv@after
                             1487
                             1488
                                   \endgroup
                             1489 }
                             The next token on the input stack is saved into \nmv@citex@next, after gobbling
      \nmv@citex@get@next
          \nmv@citex@next
                             up one token.
                             1490 \newcommand*\nmv@citex@get@next[1]{%
                                   \futurelet\nmv@citex@next\nmv@citex@punct
                             1491
                             1492 }
                             The working macro for moving the punctuation. This is very much like \@citey
         \nmv@citex@punct
\nmv@citex@punct@undouble
                             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{%

\nmv@citex@loop

```
\let\nmv@citex@loop\nmv@citex@end
                            \ifx\nmv@citex@next.\relax
                      1495
                              \ifnum\spacefactor<\nmv@citex@sfac\else
                      1496
                                \expandafter\expandafter\expandafter\nmv@citex@punct@undouble
                      1497
                      1498
                           \fi
                      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
                      1505
                      1506 }
                      1507 \newcommand*\nmv@citex@loop{}
                      The final part of the punctuation moving system.
\nmv@citex@punct@aux
                      1508 \newcommand*\nmv@citex@punct@aux[1]{%
                           \ifx\nmv@citex@next#1\@empty
                      1509
                      1510
                              \let\nmv@citex@loop\nmv@citex@get@next
                      1511
                      1512
                            \ifx#1\@nil\else
                      1513
                              \expandafter\nmv@citex@punct@aux
                      1514
                           \fi
                      1515
                      1516 }
                      The value of the spacing factor after a full stop is used to signal doubled punctu-
     \nmv@citex@sfac
                      ation. For French spacing, a bit of patching is needed.
                      1517 \mathchardef\nmv@citex@sfac3000\relax
                      \frenchspacing
                      1519
                           \mathchardef\nmv@citex@sfac1001\relax
                      1520
                           \sfcode'\.\nmv@citex@sfac
                      1521
                           \sfcode'\?\nmv@citex@sfac
                      1522
                           \sfcode'\!\nmv@citex@sfac
                      1523
                      1524 }
                      _{1525} \simeq \c \c
                      1526 \frenchspacing
                      1527 \fi
                      The swap has to be done at the beginning of the document. The internal flag
      \nmv@citex@nat
       \nmv@activate
                      from natbib is used, but under the circumstances we should be safe. \cite is also
                      patched to make the system active.
                      1528 \newcommand*\nmv@citex@nat{}
                      1529 \newcommand*\nmv@activate{%
                           \let\nmv@citex@nat\@citex
                      1530
                           \let\@citex\nmv@citex
                      1531
                           \let\nmv@cite\cite
                      1532
                           \renewcommand*{\cite}[2][]{%
                      1533
                              \nmv@ifmtarg{##1}{%
                      1534
                                \nmv@citetrue
                      1535
                                \nmv@cite{##2}%
                      1536
                      1537
```

\nmv@citefalse

1538

```
1539 \nmv@cite[##1]{##2}}%
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
1546
        \fi
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 \langle /natmove\rangle
```

8.8 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}
1559 [2020-07-21 v3.13b 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 [2020-07-21 v3.13b 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}
      [2020-07-21 v3.13b achemso configuration: ACS Appl. Energy Mater.]
1573 \def\acs@type@list{article,letter,suppinfo}
1574 \setkeys{acs}{keywords = true}
1575 (/aaemcq)
_{1576} \langle *aamick \rangle
1577 \ProvidesFile{achemso-aamick.cfg}
1578 [2020-07-21 v3.13b 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 [2020-07-21 v3.13b 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 [2020-07-21 v3.13b achemso configuration: ACS Appl. Polym. Mater.]
1591 \def\acs@type@list{article,letter,suppinfo}
1592 \setkeys{acs}{keywords = true}
1593 (/aapmcd)
_{1594} \langle *aastgj \rangle
1595 \ProvidesFile{achemso-aastgj.cfg}
1596 [2020-07-21 v3.13b achemso configuration: ACS Agri. Sci. Tech.]
1597 \def\acs@type@list{account,article,letter,retraction,review,viewpoint,suppinfo}
1598 \setkeys{acs}{keywords = true}
1599 (/aastgj)
1600 (*abseba)
1601 \ProvidesFile{achemso-abseba.cfg}
1602 [2020-07-21 v3.13b achemso configuration: ACS Biomater. Sci. Eng.]
1603 \setkeys{acs}{keywords = true}
1604 \def\acs@type@list{article,review,suppinfo}
1605 (/abseba)
1606 (*accacs)
1607 \ProvidesFile{achemso-accacs.cfg}
1608 [2020-07-21 v3.13b achemso configuration: ACS Catal.]
1609 \setkeys{acs}{keywords = true}
1610 \def\acs@type@list{article,letter,perspective,review,viewpoints,suppinfo}
1611 \SectionNumbersOff
1612 (/accacs)
1613 (*acscii)
1614 \ProvidesFile{achemso-acscii.cfg}
1615 [2020-07-21 v3.13b achemso configuration: ACS Central Sci.]
1616 \def\acs@type@list{article,review,suppinfo}
1617 \setkeys{acs}{doi = true}
1618 \SectionNumbersOff
1619 (/acscii)
1620 (*acbcct)
1621 \ProvidesFile{achemso-acbcct.cfg}
1622 [2020-07-21 v3.13b achemso configuration: ACS Chem. Biol.]
1623 \setkeys{acs}{
1624 biblabel = fullstop,
1625 biochem = true,
              = false
1626 super
1627 }
1628 \def\acs@type@list{article,letter,review,suppinfo}
1629 \SectionNumbersOff
1630 (/acbcct)
1631 (*acncdm)
1632 \ProvidesFile{achemso-acncdm.cfg}
1633 [2020-07-21 v3.13b achemso configuration: ACS Chem. Neurosci.]
1634 \def\acs@type@list{article,review,letter,suppinfo,viewpoint}
```

```
1635 \setkeys{acs}{
1636 biblabel = fullstop,
1637 biochem = true,
1638 keywords = true,
1639 super
              = false
1640 }
1641 (/acncdm)
1642 (*acsccc)
1643 \ProvidesFile{achemso-acsccc.cfg}
1644 [2020-07-21 v3.13b achemso configuration: ACS Combinatorial Sci.]
1645 \def\acs@type@list{article,letter,review,perspective,account,note,suppinfo}
1646 \setkeys{acs}{keywords = true}
1647 \SectionNumbersOff
1648 (/acsccc)
1649 (*aesccq)
1650 \ProvidesFile{achemso-aesccq.cfg}
1651 [2020-07-21 v3.13b achemso configuration: ACS Earth Space Chem.]
1652 \def\acs@type@list{article,suppinfo}
1653 \setkeys{acs}{keywords = true}
1654 (/aesccq)
1655 (*aelccp)
1656 \ProvidesFile{achemso-aelccp.cfg}
1657 [2020-07-21 v3.13b achemso configuration: ACS Energy Lett.]
1658 \def\acs@type@list{letter,perspective,review,viewpoint,focus}
1659 \SectionsOff
1660 (/aelccp)
1661 (*aeecco)
1662 \ProvidesFile{achemso-aeecco.cfg}
1663 [2020-07-21 v3.13b achemso configuration: ACS ES&T Eng.]
1664 \def\acs@type@list{article,feature,perspective,review,viewpoint}
1665 (/aeecco)
1666 (*aewcaa)
1667 \ProvidesFile{achemso-aewcaa.cfg}
1668 [2020-07-21 v3.13b achemso configuration: ACS ES&T Water]
1669 \def\acs@type@list{article,feature,perspective,review,viewpoint}
1670 (/aewcaa)
1671 (*afsthl)
1672 \ProvidesFile{achemso-afsthl.cfg}
1673 [2020-07-21 v3.13b achemso configuration: ACS Food Sci. Tech.]
1674 \def\acs@type@list{account,article,perspective,retraction,review,viewpoint}
1675 \setkeys{acs}{keywords = true}
_{1676}\left\langle /\,\mathsf{afsthl}\right\rangle
<sub>1677</sub> (*ascefj)
1678 \ProvidesFile{achemso-ascefj.cfg}
1679 [2020-07-21 v3.13b achemso configuration: ACS Infect. Dis.]
1680 \def\acs@type@list{article,letter,perspective,review,viewpoint,suppinfo}
1681 \setkeys{acs}{keywords = true}
1682 \SectionsOff
1683 (/ascefj)
1684 (*amlccd)
1685 \ProvidesFile{achemso-amlccd.cfg}
1686 [2020-07-21 v3.13b achemso configuration: ACS Macro Lett.]
1687 \def\acs@type@list{letter,suppinfo}
1688 \SectionsOff
```

```
1689 \setlength{\acs@tocentry@height}{8 cm}
1690 \setlength{\acs@tocentry@width}{4 cm}
1691 (/amlccd)
1692 (*amlcef)
1693 \ProvidesFile{achemso-amlcef.cfg}
1694 [2020-07-21 v3.13b achemso configuration: ACS Mater. Lett.]
1695 \def\acs@type@list{letter,perspective,review,viewpoint,focus}
1696 \SectionsOff
1697 (/amlcef)
1698 (*amclct)
1699 \ProvidesFile{achemso-amclct.cfg}
1700 [2020-07-21 v3.13b achemso configuration: ACS Med. Chem. Lett.]
1701 \def\acs@type@list{article,letter,perspective,suppinfo}
1702 \SectionNumbersOff
1703 (/amclct)
1704 (*amrcda)
1705 \ProvidesFile{achemso-amrcda.cfg}
1706 [2020-07-21 v3.13b achemso configuration: Acc. Mater. Res.]
1707 \def\acs@type@list{account,article,editorial,retraction,suppinfo}
1708 (/amrcda)
1709 (*ancac3)
1710 \ProvidesFile{achemso-ancac3.cfg}
1711 [2020-07-21 v3.13b achemso configuration: ACS Nano]
_{1712} \text{setkeys{acs}} \{
1713 abbreviations = true,
1714 biblabel = fullstop,
1715 etalmode = truncate,
1716 maxauthors = 20,
1717 keywords
                  = true
1718 }
1719 \def\acs@type@list{article,perspective,suppinfo}
1720 \newcommand*{\latin}[1]{\emph{#1}}
1721 \SectionNumbersOff
<sub>1722</sub> (/ancac3)
1723 (*acsodf)
1724 \ProvidesFile{achemso-acsodf.cfg}
1725 [2020-07-21 v3.13b achemso configuration: ACS Omega.]
1726 \def\acs@type@list{article}
1727 (/acsodf)
1728 (*apchd5)
1729 \ProvidesFile{achemso-apchd5.cfg}
1730 [2020-07-21 v3.13b achemso configuration: ACS Photon.]
1731 \def\acs@type@list{article,letter,perspective,review,suppinfo}
_{1732} \text{\ensuremath{\mbox{\sc true}}} \
1733 \ifx\acs@manuscript\acs@manuscript@letter
1734 \SectionNumbersOff
1735 \fi
1736 (/apchd5)
<sub>1737</sub> (*aidcbc)
1738 \ProvidesFile{achemso-aidcbc.cfg}
1739 [2020-07-21 v3.13b achemso configuration: ACS Sensors]
1740 \def\acs@type@list{article,letter,perspective,review,suppinfo}
1741 \setkeys{acs}{keywords = true}
1742 \SectionNumbersOff
```

```
1743 (/aidcbc)
1744 (*ascecg)
1745 \ProvidesFile{achemso-ascecg.cfg}
1746 [2020-07-21 v3.13b achemso configuration: ACS Sustainable Chem Eng.]
1747 \setkeys{acs}{
1748 biblabel = fullstop,
1749 keywords = true
1750 }
1751 \SectionNumbersOff
1752 \def\acs@type@list{article,feature,letter,perspective,review,suppinfo}
1753 (/ascecg)
<sub>1754</sub> (*asbcd6)
1755 \ProvidesFile{achemso-asbcd6.cfg}
_{1756} [2020-07-21 v3.13b achemso configuration: ACS Synth. Biol.]
1757 \setkeys{acs}{
1758 abbreviations = true,
     biblabel
                    = fullstop,
1759
     biochem
                    = true,
1760
1761
     keywords
                    = true,
1762 super
                     = false
1763 }
{\tt 1764 \setminus def \setminus acs@type@list\{article, letter, note, tutorial, review, suppinfo\}}
_{1765} \langle / asbcd6 \rangle
1766 (*ancham)
1767 \ProvidesFile{achemso-ancham.cfg}
1768 [2020-07-21 v3.13b achemso configuration: Anal. Chem.]
1769 \def\acs@type@list{article,note,suppinfo}
1770 \SectionNumbersOff
1771 (/ancham)
1772 (*bichaw)
1773 \ProvidesFile{achemso-bichaw.cfg}
1774 [2020-07-21 v3.13b achemso configuration: Biochemistry]
1775 \setkeys{acs}{
1776 abbreviations = true,
1777 biblabel = brackets,
1778
     biochem
                     = true,
1779 }
1780 \SectionNumbersOff
1781 \def\acs@maketitle@extras@hook{%
1782 \par
     \acs@title@short@print
1783
1784 }
_{1785} \gOaddtoOmacro{\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.

```
1786 \def\acs@author@fnsymbol#1{%
1787  \ensuremath{\%}
1788  \ifcase #1 *\or
1789  \dagger\or
1790  \ddagger\or
1791  \S\or
1792  \parallel\or
1793  \perp\or
```

```
\P\or
1794
                       \|\or
1795
                         \bot\or
1796
                            \#\or
1797
                              @\or
1798
                                \triangle\or
1799
                                  \nabla\else
1800
1801
                                    #1%
1802
        \fi
     }%
1803
1804 }
1805 \def\@maketitle@title@hook{%
     \ifnum\acs@footnote@cnt>\@ne
1806
1807
        \global\acs@footnote@cnt\@ne
1808
1809
     \fi
1810 }
1811 (/bichaw)
1812 (*bcches)
1813 \ProvidesFile{achemso-bcches.cfg}
1814 [2020-07-21 v3.13b achemso configuration: Bioconjugate Chem.]
1815 \setkeys{acs}{
1816 biochem = true,
     super = false
1817
1818 }
1819 \SectionNumbersOff
_{1820} \langle /bcches \rangle
1821 (*bomaf6)
1822 \ProvidesFile{achemso-bomaf6.cfg}
1823 [2020-07-21 v3.13b achemso configuration: Biomacromolecules]
1824 \def\acs@type@list{article,comment,communication,note,review,suppinfo}
1825 \SectionNumbersOff
1826 \AtEndOfClass{\SectionsOn}
1827 (/bomaf6)
1828 (*crtoec)
1829 \ProvidesFile{achemso-crtoec.cfg}
1830 [2020-07-21 v3.13b achemso configuration: Chem. Res. Toxicol.]
1831 \setkeys{acs}{
1832 abbreviations = true,
1833 biochem
                    = true,
1834 keywords
1835 }
1836 \def\acs@maketitle@extras@hook{%
    \par
     \acs@title@short@print
1838
1839 }
1840 \def\acs@type@list{%
1841 article, perspective, profile, review, suppinfo%
1842 }
1843 \SectionNumbersOff
1844 (/crtoec)
1845 (*chreay)
1846 \ProvidesFile{achemso-chreay.cfg}
```

```
1847 [2020-07-21 v3.13b achemso configuration: Chem. Rev.]
1849 \def\acs@type@list{review}
The references section is numbered in Chem. Rev.
1850 \def\bibsection{\acs@section{\refname}}
1851 (/chreay)
1852 (*cmatex)
        \begin{macrocode}
1853 %
1854 \ProvidesFile{achemso-cmatex.cfg}
1855 [2020-07-21 v3.13b achemso configuration: Chem. Mater.]
1856 \setkeys{acs}{keywords = true}
1857 \SectionNumbersOff
1858 \ifx\acs@manuscript\acs@manuscript@communication
1859 \AbstractOff
1860 \SectionsOff
1861\fi
1862 (/cmatex)
1863 (*cgdefu)
1864 \ProvidesFile{achemso-cgdefu.cfg}
1865 [2020-07-21 v3.13b achemso configuration: Cryst. Growth Des.]
1866 \def\acs@type@list{%
1867 article, communication, perspective, suppinfo%
1868 }
1869 \SectionNumbersOff
1871 \SectionsOff
1872 \fi
1873 \setlength{\acs@tocentry@height}{8.9 cm}
1874 \setlength{\acs@tocentry@width}{4.6 cm}
1875 (/cgdefu)
1876 (*enfuem)
1877 \ProvidesFile{achemso-enfuem.cfg}
1878 [2020-07-21 v3.13b achemso configuration: Energy Fuels]
1879 \def\acs@type@list{article,review,suppinfo}
1880 \SectionNumbersOff
1881 (/enfuem)
1882 (*esthag)
1883 \ProvidesFile{achemso-esthag.cfg}
1884 [2020-07-21 v3.13b achemso configuration: Environ. Sci. Technol.]
1885 \def\acs@type@list{article,suppinfo}
1886 \SectionNumbersOff
1887 (/esthag)
1888 (*estlcu)
1889 \ProvidesFile{achemso-estlcu.cfg}
_{1890} [2020-07-21 v3.13b achemso configuration: Environ. Sci. Technol. Lett.]
1891 \def\acs@type@list{letter,suppinfo}
1892 \SectionNumbersOff
1893 (/estlcu)
1894 (*iecred)
1895 \ProvidesFile{achemso-iecred.cfg}
1896 [2020-07-21 v3.13b achemso configuration: Ind. Eng. Chem. Res.]
1897 \setkeys{acs}{biblabel = brackets}
1898 \SectionNumbersOff
```

```
1899 (/iecred)
1900 (*inoraj)
1901 \ProvidesFile{achemso-inoraj.cfg}
1902 [2020-07-21 v3.13b achemso configuration: Inorg. Chem.]
1903 \SectionNumbersOff
1904 \ifx\acs@manuscript\acs@manuscript@communication
1905 \AbstractOff
1906 \SectionsOff
1907\fi
1908 \setkeys{acs}{doi = true}
1909 (/inoraj)
1910 (*jafcau)
1911 \ProvidesFile{achemso-jafcau.cfg}
1912 [2020-07-21 v3.13b achemso configuration: J. Agric. Food Chem.]
1913 \setkeys{acs}{keywords = true}
1914 \def\acs@type@list{article,suppinfo}
1915 \SectionNumbersOff
1916 (/jafcau)
1917 (*jceda8)
1918 \ProvidesFile{achemso-jceda8.cfg}
1919 [2020-07-21 v3.13b achemso configuration: J. Chem. Ed.]
1920 \setkeys{acs}{keywords = true}
1921 \SectionNumbersOff
1922 \def\acs@type@list{article,suppinfo}
1923 \SectionNumbersOff
1924 (/jceda8)
1925 (*jceaax)
1926 \ProvidesFile{achemso-jceaax.cfg}
1927 [2020-07-21 v3.13b achemso configuration: J. Chem. Eng. Data]
1928 \def\acs@type@list{article,suppinfo}
1929 \def\refname{Literature Cited}
1930 \SectionNumbersOff
1931 (/jceaax)
1932 (*jcisd8)
1933 \ProvidesFile{achemso-jcisd8.cfg}
1934 [2020-07-21 v3.13b achemso configuration: J. Chem. Inf. Model.]
1935 \def\acs@type@list{article,suppinfo}
1936 \SectionNumbersOff
1937 (/jcisd8)
1938 (*jctcce)
1939 \ProvidesFile{achemso-jctcce.cfg}
1940 [2020-07-21 v3.13b achemso configuration: J. Chem. Theory Comput.]
1941 \def\acs@type@list{article,suppinfo}
1942 \setkeys{acs}{maxauthors = 0}
1943 (/jctcce)
1944 (*jmcmar)
1945 \ProvidesFile{achemso-jmcmar.cfg}
1946 [2020-07-21 v3.13b achemso configuration: J. Med. Chem.]
1947 \def\acs@type@list{article,letter,perspective,suppinfo}
1948 \SectionNumbersOff
1949 \setlength{\acs@tocentry@height}{5.5cm}
1950 \setlength{\acs@tocentry@width}{21cm}
1951 (/jmcmar)
1952 (*jnprdf)
```

```
1953 \ProvidesFile{achemso-jnprdf.cfg}
1954 [2020-07-21 v3.13b achemso configuration: J. Nat. Prod.]
1955 \renewcommand*{\abstractname}{ABSTRACT}
1957 \renewcommand*{\suppinfoname}{ASSOCIATED CONTENT}
1958 \SectionNumbersOff
1959 \renewcommand*{\acs@abstract}{%
     \quotation
1961 \textbf{\abstractname :}%
1962 }
1963 \AbstractOn
1964 \ifx\acs@manuscript\acs@manuscript@communication
1965 \AbstractOff
     \SectionsOff
1966
1967\fi
1968 \def\refname{REFERENCES}
1969 \captionsetup{
1970 labelfont = bf,
1971 labelsep = period
1972 }
1973 (/jnprdf)
1974 (*joceah)
1975 \ProvidesFile{achemso-joceah.cfg}
1976 [2020-07-21 v3.13b achemso configuration: J. Org. Chem.]
1977 \ifx\acs@manuscript\acs@manuscript@communication
1978 \AbstractOff
1979 \SectionsOff
1980 \fi
1981 \floatstyle{plaintop}
1982 \restylefloat{scheme}
1983 \floatstyle{plain}
1984 \renewcommand*\acs@type@list{article,communication,note,perspective,review,suppinfo}
1985 (/joceah)
1986 (*jpcafh)
1987 \ProvidesFile{achemso-jpcafh.cfg}
1988 [2020-07-21 v3.13b achemso configuration: J. Phys. Chem. A]
1989 \def\acs@type@list{article,suppinfo}
1990 \setkeys{acs}{
1991 etalmode
                  = truncate,
1992 maxauthors = 10
1993 }
1994 \SectionNumbersOff
1995 \captionsetup[table] {labelfont=bf,textfont=bf}
1996 \g@addto@macro{\maketitle}{\newpage}
1997 (/jpcafh)
1998 (*jpcbfk)
1999 \ProvidesFile{achemso-jpcbfk.cfg}
2000 [2020-07-21 v3.13b achemso configuration: J. Phys. Chem. B]
2001 \def\acs@type@list{article,suppinfo}
2002 \setkeys{acs}{
                  = truncate,
2003 etalmode
2004 maxauthors = 10
```

```
2005 }
2006 \SectionNumbersOff
2007 \captionsetup[table]{labelfont=bf,textfont=bf}
2008 \g@addto@macro{\maketitle}{\newpage}
2009 (/jpcbfk)
2010 (*jpccck)
2011 \ProvidesFile{achemso-jpccck.cfg}
     [2020-07-21 v3.13b achemso configuration: J. Phys. Chem. C]
2013 \def\acs@type@list{article,suppinfo}
2014 \setkeys{acs}{
2015 etalmode
                   = truncate,
    maxauthors = 10
2016
2017 }
2018 \SectionNumbersOff
2019 \captionsetup[table] {labelfont=bf, textfont=bf}
2020 \g@addto@macro{\maketitle}{\newpage}
2021 (/jpccck)
2022 (*jpclcd)
2023 \ProvidesFile{achemso-jpclcd.cfg}
_{2024} [2020-07-21 v3.13b achemso configuration: J. Phys. Chem. Lett.]
2025 \setkeys{acs}{
2026 etalmode
                = truncate,
     maxauthors = 10
2027
2028 }
2029 \def\acs@type@default{letter}
2030 \def\acs@type@list{letter}
2031 \SectionNumbersOff
2032 \captionsetup[table]{labelfont=bf,textfont=bf}
2033 \g@addto@macro{\maketitle}{\newpage}
2034 \renewcommand{\acs@tocentry@print}[1]{%
     \gdef\acs@tocentry@text{#1}%
2035
2036 }
2037 \renewcommand*{\acs@abstract@extras}{%
     \begingroup
2038
        \acs@tocentry@print@aux
2039
      \endgroup
2040
     \acs@keywords@print
2041
     \newpage
2042
2043 }
2044 \setlength\acs@tocentry@height{2in}
2045 \setlength\acs@tocentry@width{2in}
2046 (/jpclcd)
2047 (*jprobs)
2048 \ProvidesFile{achemso-jprobs.cfg}
2049 [2020-07-21 v3.13b achemso configuration: J. Proteome Res.]
2050 \setkeys{acs}{keywords = true}
2051 \def\acs@type@list{article,review,suppinfo}
2052 \SectionNumbersOff
2053 (/jprobs)
The J. Am. Chem. Soc. configuration is rather more complicated as there is the
need to construct a "galley-like" layout for communications.
2055 \ProvidesFile{achemso-jacsat.cfg}
```

```
2056 [2020-07-21 v3.13b achemso configuration: J. Am. Chem. Soc.]
            2057 \SectionNumbersOff
            2059 \expandafter\endinput
            2060 \fi
            2061 \setkeys{acs}{articletitle = true}
            Everything from here onward applies only to communications. Some adjustments
            are now made using the existing tools.
            2062 \setkeys{acs}{
            2063 email = true,
                 layout = twocolumn
            2064
            2065 }
            2066 \SectionsOff
            2067 \acs@layout@nine
           The abstract appears at the start of the document, with lines around it.s
   abstract
            2068 \renewenvironment{abstract}{%
                 \hrule
            2069
                 \vspace{2 mm}%
            2070
            2071 \sffamily
            2072 \noindent
            2073 \emph{\textbf{Abstract:}}%
            2074 }{%
            2075 \vspace{2 mm}%
            2076 \hrule
            2077 \vspace{6 mm}%
            2078 }
   \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 2079 \def\affilsize{%
\emailsize 2080
                 \@setfontsize\affilsize\@ixpt\@xpt
  \capsize 2081 }
  \refsize 2082 \def\acksize{%
 \suppsize 2083
                 \@setfontsize\acksize\@ixpt\@xipt
\titlesize 2084}
            _{2086} \@setfontsize\authorsize{10.5}{12.5}%
            2087 }
            2088 \newcommand*\capsize{%
            2089 \@setfontsize\capsize\@viiipt\@ixpt
            2090 }
            2091 \def\emailsize{%
            2092 \@setfontsize\emailsize\@viiipt{15}%
            2093 }
            2094 \newcommand*\refsize{%
            2095 \@setfontsize\refsize{7.5}{7.5}%
            2096 }
            2097 \def\suppsize{%
            2098 \@setfontsize\suppsize{8.5}{10.5}\%
            2099 }
            2100 \def\titlesize{%
            2101 \@setfontsize\titlesize\@xiipt{13}%
```

```
2102 }
                           2103 \let\footnotesize\refsize
                           2104 \let\captionfont\capsize
              \emailfont
                          A slight font change.
                           2105 \def\emailfont{\sffamily}
                           The header styles are done the hard way, to keep down the number of packages
               \ps@plain
                \ps@jacs
                           loaded.
                           2106 \def\ps@plain{%
                                 \let\@mkboth\@gobbletwo
                           2107
                                 \let\@oddhead\@empty
                           2108
                                 \def\@oddfoot{%
                           2109
                                   \reset@font
                           2110
                                   \sffamily
                           2111
                                   \textbf{\thepage}%
                           2112
                                   \hfil
                           2113
                           2114
                                 }%
                           2115
                                 \let\@evenhead\@empty
                           2116
                                 \let\@evenfoot\@oddfoot
                           2117 }
                           2118 \ensuremath{\mbox{def\ps@acs}{\mbox{\%}}}
                                 \def\@oddfoot{%
                           2119
                                   \reset@font
                           2120
                                   \sffamily
                           2121
                                   \textbf{\thepage}%
                           2122
                                   \hfil
                           2123
                                 ጉ%
                           2124
                                 \def\@evenfoot{%
                           2125
                           2126
                                   \reset@font
                                   \hfil
                           2127
                                   \sffamily
                           2128
                                   \textbf{\thepage}%
                           2129
                                 }%
                           2130
                                 \def\@oddhead{}%
                           2131
                                 \let\@evenhead\@oddhead
                           2132
                           2133 }
                           2134 \pagestyle{acs}
                           Length adjustments for the title.
   \acs@space@pre@title
  \acs@space@post@title
                           2135 \setlength\acs@space@pre@title{16mm}
 \acs@space@post@author
                           2136 \setlength\acs@space@post@title{Omm}
\acs@space@post@address
                           2137 \setlength\acs@space@post@author{Omm}
                           2138 \setlength\acs@space@post@address{0mm}
 \acs@space@post@email
                           2139 \setlength\acs@space@post@email{-1mm}
                           2140 \setlength\acs@maketitle@width{152.4mm}
   \acs@contact@details
                         Contact details are different here.
                           2141 \def\acs@contact@details{%
                                Received \today; E-mail: \acs@email@list
                           2142
                           2143 }
                           No keywords or abbreviations for J. Am. Chem. Soc..
 \acs@maketitle@extras
```

2144 \let\acs@maketitle@extras\relax

```
Getting the floats correct is a difficult task "by hand"; using the caption package
makes this a lot easier.
2145 \floatstyle{plaintop}
```

```
2146 \restylefloat{scheme}
2147 \floatstyle{plain}
2148 \DeclareCaptionLabelSeparator{perquad}{.\quad}
2149 \captionsetup{
2150 singlelinecheck = off,
2151
     labelfont
                     = {bf,it,sf},
2152
     textfont
                      = sf,
2153
     labelsep
                      = perquad
2154 }
2155 \captionsetup[figure] {textfont=rm}
```

\acs@table A patch or \table.

```
2157 \let\acs@table\table
       2158 \left\lceil \frac{1}{2} \right\rceil
            \capsize
       2159
       2160
            \acs@table
       2161 }
```

The bibliography has to be adjusted.

```
2162 \AtBeginDocument{%
2163 \def\bibsection{%
       \@startsection
2164
2165
         {section}
2166
          {1}
          {z0}{z0}{2.5mm}%
2167
          {\normalfont\acksize\bfseries}
2168
          {\hrule\nobreak\vspace{1.2mm}\noindent\refname}%
2169
     }%
2170
     \let\bibfont\refsize
2171
     \setlength{\bibhang}{0.61cm}%
2172
     \setlength{\bibsep}{0mm}%
2173
2174 }
2175 (/jacsat)
2176 (*langd5)
2177 \ProvidesFile{achemso-langd5.cfg}
2178 [2020-07-21 v3.13b achemso configuration: Langmuir]
2179 \def\acs@type@list{article,letter,suppinfo}
2180 \SectionNumbersOff
2181 (/langd5)
2182 (*mamobx)
2183 \ProvidesFile{achemso-mamobx.cfg}
2184 [2020-07-21 v3.13b achemso configuration: Macromolecules]
2185 \SectionNumbersOff
2186 \setkeys{acs}{doi = true}
2187 (/mamobx)
2188 (*mpohbp)
2189 \ProvidesFile{achemso-mpohbp.cfg}
2190 [2020-07-21 v3.13b achemso configuration: Mol. Pharm.]
2191 \setkeys{acs}{keywords = true}
2192 \def\acs@type@list{article,suppinfo}
```

```
2193 \SectionNumbersOff
_{2194}\left</\mathsf{mpohbp}\right>
_{2195} (*nalefd)
2196 \ProvidesFile{achemso-nalefd.cfg}
2197 [2020-07-21 v3.13b achemso configuration: Nano Lett.]
2198 \setkeys{acs}{keywords = true}
2199 \def\acs@type@default{letter}
2200 \def\acs@type@list{letter}
2201 \SectionNumbersOff
_{2202} \langle / nalefd \rangle
2203 (*orlef7)
2204 \ProvidesFile{achemso-orlef7.cfg}
2205 [2020-07-21 v3.13b achemso configuration: Org. Lett.]
2206 \def\acs@type@default{communication}
2207 \def\acs@type@list{communication}
2208 \SectionNumbersOff
2209 \setkeys{acs}{layout = twocolumn}
2210 \RequirePackage{xcolor}
{\tt 2211} \verb| definecolor{orglett}{RGB}{128,0,0}|
2212 (/orlef7)
2213 (*oprdfk)
2214 \ProvidesFile{achemso-oprdfk.cfg}
2215 [2020-07-21 v3.13b achemso configuration: Org. Proc. Res. Dev.]
2216 \def\acs@type@list{article,highlight,review,suppinfo}
2217 \SectionNumbersOff
2218 (/oprdfk)
2219 (*orgnd7)
2220 \ProvidesFile{achemso-orgnd7.cfg}
     [2020-07-21 v3.13b achemso configuration: Organometallics]
2222 \SectionNumbersOff
2223 (/orgnd7)
```

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10 References

- [1] This note text will be in the bibliography.
- [2] Coghill, A. M., Garson, L. R., Eds. *The ACS Style Guide*, 3rd ed.; Oxford University Press, Inc. and The American Chemical Society: New York, 2006.