

A demonstration of the `achemso` \LaTeX class

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Abstract

This is an example document for the `achemso` document class, intended for submissions to the American Chemical Society for publication. The class is based on the standard \LaTeX 2 ϵ report file, and does not seek to reproduce the appearance of a published paper.

This is an abstract for the `achemso` document class demonstration document. An abstract is only allowed for certain manuscript types. The selection of `journal` and `manuscript` will determine if an abstract is valid. If not, the class will issue an appropriate error.

Introduction

This is a paragraph of text to fill the introduction of the demonstration file. The demonstration file attempts to show the modifications of the standard \LaTeX macros that are implemented by the `achemso` class. These are mainly concerned with content, as opposed to appearance.

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Results and discussion

Outline

The document layout should follow the style of the journal concerned. Where appropriate, sections and subsections should be added in the normal way. If the class options are set correctly, warnings will be given if these should not be present.

References

The class makes various changes to the way that references are handled. The class loads natbib, and also the appropriate bibliography style. References can be made using the normal method; the citation should be placed before any punctuation, as the class will move it if using a superscript citation style.^{1,2} The use of natbib allows the use of the various citation commands of that package: Abernethy et al. have shown something, in 1999, or as given by Ref. 1. Long lists of authors will be automatically truncated in most article formats, but not in supplementary information or reviews.⁴ If you encounter problems with the citation macros, please check that your copy of natbib is up to date.

Multiple citations to be combined into a list can be given as a single citation. This uses the mciteplus package.⁵ Citations other than the first of the list should be indicated with a star. If the mciteplus package is not installed, the standard bibliography tools will still work but starred references will be ignored.

The class also handles notes to be added to the bibliography. These should be given in place in the document.⁶ As with citations, the text should be placed before punctuation. A note is also generated if a citation has an optional note. This assumes that the whole work has already been cited: odd numbering will result if this is not the case.⁷

Floats

New float types are automatically set up by the class file. The means graphics are included as follows (Scheme 1). As illustrated, the float is “here” if possible.

Your scheme graphic would go here: `.eps` format
for `LATEX` or `.pdf` (or `.png`) for `pdfLATEX`
CHEMDRAW files are best saved as `.eps` files;
these can be scaled without loss of quality, and can be
converted to `.pdf` files easily using `eps2pdf`.

Scheme 1: An example scheme

As well as the standard float types `table`
and `figure`, the class also recognises
`scheme`, `chart` and `graph`.

Figure 1: An example figure

Charts, figures and schemes do not necessarily have to be labelled or captioned. However, tables should always have a title. It is possible to include a number and label for a graphic without any title, using an empty argument to the `\caption` macro.

The use of the different floating environments is not required, but it is intended to make document preparation easier for authors. In general, you should place your graphics where they make logical sense; the production process will move them if needed.

Math(s)

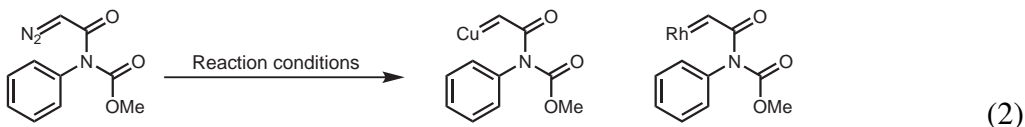
The `achemso` class does not load any particular additional support for mathematics. If the author *needs* things like `amsmath`, they should be loaded in the preamble. However, the basics should work fine. Some inline material $y = mx + c$ followed by some display.

$$A = \pi r^2$$

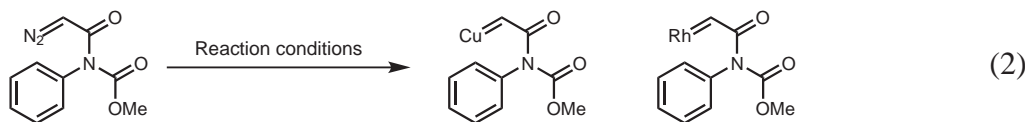
It is possible to label equations in the usual way.

$$\frac{d}{dx}r^2 = 2r \quad (1)$$

This can also be used to have equations containing graphical content. Just need to have graphic (`nice.eps`) and equation number aligned.



This is how I want it (`ugly.eps`) = a lot of workarounds.



There is a invisible (white) frame around the reaction as wide as document body to have the number (entered in ChemDraw) aligned to the right and reaction scheme centered. No cross referencing possible. Please help!

Experimental

The usual experimental details should appear here. This could include a table, which can be referenced as Table 1. Notice that the caption is positioned at the top of the table. Do not worry about the appearance of the table: this will be altered during production.

Adding notes to tables can be complicated. Perhaps the easiest method is to generate these using the basic `\textsuperscript` and `\emph` macros, as illustrated (Table 2).

The example file also loads the `mhchem` package, so that formulas are easy to input: `\{H2SO4\}` gives H_2SO_4 . See the use in the bibliography file (when using titles in the references section).

Table 1: An example table

Header one	Header two
Entry one	Entry two
Entry three	Entry four
Entry five	Entry five
Entry seven	Entry eight

Table 2: A table with notes

Header one	Header two
Entry one ^a	Entry two
Entry three ^b	Entry four

^a Some text; ^b Some more text.

The use of new commands should be limited to simple things which will not interfere with the production process. For example, `\mycommand` has been defined in this example, to give italic, monospaced text: *some text*.

Extra information when writing JACS Communications

When producing communications for *J. Am. Chem. Soc.*, the class will automatically lay the text out in the style of the journal. This gives a guide to the length of text that can be accommodated in such a publication. There are some points to bear in mind when preparing a JACS Communication in this way. The layout produced here is a *model* for the published result, and the outcome should be taken as a *guide* to the final length. The spacing and sizing of graphical content is an area where there is some flexibility in the process. You should not worry about the space before and after graphics, which is set to give a guide to the published size. This is very dependant on the final published layout.

You should be able to use the same source to produce a JACS Communication and a normal article. For example, this demonstration file will work with both `type=article` and `type=communication`. Sections and any abstract are automatically ignored, although you will get warnings to this effect.

Acknowledgement

Please use “The authors thank ...” rather than “The authors would like to thank ...”.

The author thanks Mats Dahlgren for version one of `achemso`, and Donald Arseneau for the code taken from `cite` to move citations after punctuation.

Supporting Information Available

This will usually read something like: “Experimental procedures and characterization data for all new compounds. This material is available free of charge via the Internet at <http://pubs.acs.org>.”

The entire `achemso` bundle is generated by running `achemso.dtx` through \TeX . Running \LaTeX on the same file will generate the general documentation for both the class and package files.

This material is available free of charge via the Internet at <http://pubs.acs.org>.

Notes and References

- (1) Abarca, A.; Gómez-Sal, P.; Martín, A.; Mena, M.; Poblet, J. M.; Yélamos, C. *Inorg. Chem.* **2000**, 39, 642–651.
- (2) Abernethy, C. D.; Codd, G. M.; Spicer, M. D.; Taylor, M. K. *J. Am. Chem. Soc.* **2003**, 125, 1128–1129.
- (3) Cotton, F. A.; Wilkinson, G.; Murillio, C. A.; Bochmann, M. *Advanced Inorganic Chemistry*, 6th ed.; Wiley: Chichester, 1999.
- (4) Frisch, M. J. et al. *Gaussian 03*; Gaussian, Inc.: Wallingford, CT, 2004.
- (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.

(6) This is a note. The text will be moved the the references section. The title of the section will change to “Notes and References”.

(7) Ref. 3, p. 1.

Graphical TOC Entry

Some journals require a graphical entry for the Table of Contents. This should be laid out "print ready" so that the sizing of the text is correct.

Inside the `tocentry` environment, the font used is Helvetica 8pt, as required by *Journal of the American Chemical Society*.

The surrounding frame is 9 cm by 3.5 cm, which is the maximum permitted for *Journal of the American Chemical Society* graphical table of content entries. The box will not resize if the content is too big: instead it will overflow the edge of the box.

This box and the associated title will always be printed on a separate page from the rest of the document. It is best to place the graphical TOC entry as the last item in the draft so that the page break is not a problem.