The rsc package — BibTeX styles and utilities for chemical documents*

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Abstract

The rsc package provides BibTeX style files to produce bibliographies in accordance with the guidelines of the Royal Society of Chemistry and Wiley chemistry-related journals. It also provides a small number of useful chemistry related functions.

1 Introduction

Although synthetic chemists do not, in the main, use LaTeX for the preparation of journal articles, it would be nice to be able to use it for reports. The package achemso provides for a BibTeX style and other support for reports in the style of the American Chemical Society. The aim of the rsc package is to provide similar support for the style favoured by the Royal Society of Chemistry. The package also provides support for the style used in Wiley-published journals.

In addition to providing the core *.bst files, this package also generates *-mc.bst, rsc.sty rsc.tex. The *-mc.bst files includes support for the mcite package, allowing the generation of multiple references. The macro collection rsc.sty provides a few useful features not catered for by other chemistry-related packages. Finally, rsc.tex is a simple template for using the BibTeX styles, including loading some other very useful chemistry packages.

2 Bibliography design decisions

Along with almost every BibTeX style file, much of the bst file design is inherited from the original BibTeX style files provided by Oren Patashnik. However, while the original styles were designed to be flexible, the style files here are designed to do a single job. Thus much of the original flexibility has been stripped out to give a clearer design. This has many be achieved by removing unused functions. The style files provided here are therefore poor examples for others to work from!

Chemistry journals give only minimal guidance on the format of references other than for journal articles. Most of the other types are therefore based on current practice in RSC and Wiley journals. Some of this is contradictory, and so I have gone with I feel is most consistent. Please e-mail me if you feel I have got things wrong!

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3 Bibliography usage information

3.1 Cross-references

Unlike most BibTeX styles, the style files provided here do not support cross-referencing between references. Using crossref will still fill in missing information, but will not output "see ref. X". Chemistry references do not lend themselves to the use of crossref.

3.2 Notes

As in pccp.bst, notes are not output for most reference types. The reasoning here is that it is difficult to predict how people will want to use notes. In chemistry, they may be used in several forms, for example:

- See for example: I. V. Gostunskaya, V. S. Petrova, A. I. Leonava, V. A. Mironava, M. Abubaker, and B. Kazanski, *Neftekhimiya*, 1967, **7**, 3–8.
- I. V. Gostunskaya, V. S. Petrova, A. I. Leonava, V. A. Mironava, M. Abubaker, and B. Kazanski, *Neftekhimiya*, 1967, **7**, 3–8 and references therein.
- I. V. Gostunskaya, V. S. Petrova, A. I. Leonava, V. A. Mironava, M. Abubaker, and B. Kazanski, *Neftekhimiya*, 1967, **7**, 3–8 (*Chem. Abs.*, 1967, **67**, 21276t).

This is pretty much impossible to handle automatically, especially as the format you want might change depending on the report you are writing. So I would recommend using the misc type, and doing the formatting by hand. If other people feel the behaviour is not the best solution, please e-mail me.

3.3 Multiple citations

By default, BibTeX does not handle producing compound references. Although it is not perfect, the package mcite allows you to produce references of the format:

K. Öfele, J. Organomet. Chem., 1968, 12, P42-P43; C. D. Abernethy, A. H. Cowley and R. A. Jones, J. Organomet. Chem., 2000, 596, 3-5.

Although the package only requires a minor modification of the BibTeX style file, it seems a good idea to provide one automatically. The *-mc.bst are produced with the necessary modifications made to *.bst. Note that this requires \usepackage{mcite} in your LaTeX source.

3.4 Additional entry types

In order to ensure compatibility with the achemso package, the non-standard entry types remark, inpress and submitted are supported. The implementation is modelled on achemso.bst, but the notes field is not used for inpress and submitted.

4 Additional macros

4.1 Overview

The macros provide by rsc.sty are all very simple. They simply fill in a few gaps in the available support for chemists in LaTeX. Most are built on other, more powerful, packages. As a result, it is best to read the documents for the "parent" package to alter the handling of the macros given here. The package follows the house style of the RSC, by default. The angew option switches to the Wiley house style, modelled on the approach taken in Angew. Chem.

4.2 Additional units

The unitsdef package provides a great number of easy to use unit commands, and handles spacing between numbers and units very well. However, it misses out a few useful units for chemistry. The unitsdef package is loaded by rsc.sty, and is then used to provide five additional units. The most obvious of these is \Hz, which simply gives Hz. The unitsdef package only defines \hertz, which is not as obvious. The command \mmHg has a non-breaking thin space, leading to mmHg. Two related commands are given for concentration: \molar gives moldm⁻³, whilst \Molar gives M. Finally, the command \cmc is provided for generating cm³. All space correctly with numbers, so inputting 10\cmc gives 10 cm³, with a non-breaking space.

\mmHg \molar \Molar \cmc

4.3 The standard state symbol

\standardstate

Related to, but not exactly a unit is the \standardstate command. This generates the tricky $^{\ominus}$ symbol, letting you put \$\Delta S \standardstate\$ to generate ΔS^{\ominus} . Note that this is safe in text and maths mode.

4.4 Alkyl radicals

\iPr \iBu \tBu There are a few alkyl radicals that come up all of the time. No one seems to have put these into a package, so they are provided here. As you would expect, \iPr gives Prⁱ, \Bu gives Buⁱ and \tBu gives Bu^t. These are in the style most commonly seen in RSC journals. The package option angew changes the format to that used in Wiley journals, so for example \iPr then gives iPr.

4.5 Floating schemes

A number of approaches can be taken to redefining all float types in a consistent manner (I know, I've tried several!). In the end, the easiest method seems to be to use an "internal" float type in the package, and then define a related environment to present to the user. As a result, this part of the package is by far the most complex.

scheme

The float package allows new float types to be defined. This is used to create a scheme environment, which works very much like the figure environment. In contrast to the LaTeX default, all float types are defined to be "here" if possible by default, then float to the top of the page. This is usually what chemists expect to happen. All the float types are also defined to take one optional argument to

over-ride the provided placement behaviour. The most likely use is to put [H] to force a float to be "here", absolutely. So for example, we might have:

```
Some text about \ref{sch1}, which will appear directly under this paragraph and will not float at all!
\begin{scheme}[H]
This is where the scheme should go%
\caption{An exciting reaction, placed HERE.}%
\label{sch1}
\end{scheme}
```

To give:

Some text about Scheme 1, which will appear directly under this paragraph and will not float at all!

This is where the scheme should go

Scheme 1 An exciting reaction, placed HERE.

In addition to providing the floats, referencing to schemes, figures and tables is formatted using the varioref package, to give references such as "Scheme 1", "Table 2", etc. from simple \ref commands.

\listofschemes

A listing command for schemes \lisofschemes, is provided in analogy to \listoffigures. It takes one optional argument to alter the title of the list. The \listoffigures and \listoftables commands are redefined to act in the same way.

A number of package options are provided to alter the handling of the floating environments. By default, the float contents are centred on the page. The option floatleft (also shortened to f1) is available to produce the standard LaTeX behaviour of left-aligned floats. Captions are also centred by default, but may be left-aligned using the captionleft (c1) option. The format of the labels once again follows the RSC or Wiley house styles. Note that the angew package option automatically sets c1 as well. Finally, schemes may be numbered within chapters by using the chapter (ch) option. This is obviously provided for theses and other very long documents.

5 A LaTeX template

This is a very simple template for chemistry-related documents. The babel system is used to give UK hyphenation. As well as the macros given in this package as rsc, the packages bpchem and mhchem are loaded, as both provide useful support for the chemist. The rsc package loads cite automatically, giving superscript citations which come after punctuation. With the angew option, these are also surrounded by square brackets.

```
1 \documentclass[12pt,a4paper]{article}
2 \usepackage[T1]{fontenc}
3 \usepackage[english,UKenglish]{babel}
4 \usepackage[version=3]{mhchem}
5 \usepackage{rsc} % Package options are angew, ch, fl and cl
```

6 BibLaTeX support

The next area of work for the rsc package is support for Philipp Lehman's new BibLaTeX system. This is in development, although currently a release date is not certain. The aim will be to reproduce the functionallity of the current BibTeX style files, taking account of the slight changes that BibLaTeX introduces in database entries.