

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`, `*nat.bst`, `rsc.sty` and `rsc.tex`. The `*-mc.bst` files includes support for the `mcite` package, allowing the generation of multiple references. The `*nat.bst` files allow the use of the `natbib` package with BibTeX style files. 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

^{*}This file describes version v2.1, last revised 2007/08/05.

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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!

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:

1. 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 natbib support

The files `rscnat.bst` and `angewnat.bst` provide support for the generation of bibliographies for use with the `natbib` package. As well as altering the `\bibliographystyle` command appropriately, you also need to load `natbib`. The `rsc` package file provides the option `natbib`, which loads `natbib` automatically (normally, `rsc` loads the `cite` package). Note that `natbib` and `mcite` are incompatible, so you must choose one or the other.

3.5 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 provided by `rsc.sty` are in the main very simple. They 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 mol dm⁻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.

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

4.5 Floats

The float management section of `rsc` has been totally rewritten in version 2. The provision of a float type for schemes is now handled by the `chemscheme` package; this is loaded automatically by `rsc`. The formatting of float types `table`, `figure` and `scheme` is modified by the `rsc` package to conform to the appropriate journal style. This also applies to cross-references and float captions. The `rsc` package will pass any options appropriate for `chemscheme` through to that package (currently, these are `chapter`¹ and `chemcompounds`²).

`\floatcontentscentre` By default, the contents of all floats are centred on the page. This behaviour
`\floatcontentsleft` may be changed globally by using the `floatleft` (or `fl`) package option. The behaviour may be changed for selected floats by issuing the command `\floatcontentscentre` or `\floatcontentsleft` *before* the beginning of the floating environment. This change remains in force until cancelled using the complementary macro. These packages are provided by the `chemscheme` package.

Single line float captions are centred by default, but may be left-aligned using the `captionleft` (`cl`) option. The `angew` option automatically activates `captionleft`, as this is the house style in Wiley journals. All multi-line captions are flush left.

4.6 Summary of options

The `rsc` package has a number of options, mainly concerned with controlling formatting. The full range of options is summarised in Table 1.

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 `mhchem` package is loaded, as it provides useful support for the chemist. The `rsc` package loads `cite` (or `natbib`) automatically, giving

¹Numbers schemes per chapter rather than globally.

²This option loads the `chemcompounds` package, instead of the default of `bpchem`. Both can be used to automatically track reference numbers given to chemical compounds. See the `chemscheme` documentation for a more detailed discussion of this option.

Table 1 Summary of `rsc` package options

Option	Effect
<code>angew</code>	Use Wiley (<i>Angew. Chem.</i>) formatting
<code>ch</code>	Number schemes within chapters (if present)
<code>chapter</code>	Number schemes within chapters (if present)
<code>chemcompounds</code>	Use <code>chemcompounds</code> package for tracking chemical numbers, rather than <code>bpchem</code>
<code>cl</code>	All captions flush left
<code>captionleft</code>	All captions flush left
<code>fl</code>	Float contents flush left
<code>floatleft</code>	Float contents flush left
<code>natbib</code>	Use <code>natbib</code> rather than <code>cite</code>

superscript citations. The `cite` package also moves citations to after punctuation. With the `angew` option, references are surrounded by square brackets.

```
1 \documentclass[a4paper]{article}
2 \usepackage[T1]{fontenc}
3 \usepackage[english,UKenglish]{babel}
4 \usepackage[version=3]{mhchem}
5 \usepackage{rsc}
6 \usepackage{mcite}           % Pick one or the other
7 %\usepackage{natbib}        % as they are incompatible
8 \begin{document}
9 \bibliography{refs}         % Your reference database
10 \bibliographystyle{rsc-mc} % Take your pick of styles
11 \end{document}
```

6 Known issues

The `memoir` class implements its own customisable float and caption management. Unfortunately, this does not have flexibility in the areas needed by the `rsc` package. As a result, the `memoir` methods are over-written with the procedures from the `float` and `caption` packages. This may cause some features to fail or behave unexpectedly. The decision to use `float` and `caption` came down to considering the aims of *this* package.

7 Future plans

The `biblatex` package, currently being developed by Phillip Lehman, is likely to become the standard for bibliography formatting in the future. However, currently package is still in beta, and the interface is not finalised. Thus at present it is too early to produce `biblatex` styles for general release.

Once biblatex reaches production, it is my intention to provide suitable support files for chemical journals. It seems likely that these will be in a separate package (probably covering a number of journal styles). At that stage, the support macros provided here may be moved to a more general purpose package. It is my aim to implement an extendable style system, to allow more convenient support for a wider range of journals. Suitable steps will be taken to maintain the user interface provided here (and in the `achemso` package).

8 The package code

The style file `rsc.bst` stands on its own, and `rsc-mc.bst` only needs the `mcite` in order to function correctly. However, a few extra commands are useful for chemists, and are not available elsewhere (to my knowledge). So this seems a good place to define them. The code is all very simple, but for the interested reader is provided here.

8.1 Setup code

First of all, the package identifies itself and loads other packages needed to function.

```
12 \NeedsTeXFormat{LaTeX2e}
13 \ProvidesPackage{rsc}[2007/08/05 v2.1
14   Useful chemistry functions]
15 \RequirePackage{unitsdef,graphicx,amssymb,fixltx2e,varioref}
```

The Boolean values needed to manage options are set up.

```
16 \newif \ifRSC@fl \RSC@flfalse
17 \newif \ifRSC@cl \RSC@clfalse
18 \newif \ifRSC@chapter \RSC@chapterfalse
19 \newif \ifRSC@angew \RSC@angewfalse
20 \newif \ifRSC@natbib \RSC@natbibfalse
```

The package provides several options which relate to float handling, plus one for `natbib` and one for *Angew. Chem.* style formatting.

```
21 \DeclareOption{floatleft}{\global\RSC@fltrue}
22 \DeclareOption{fl}{\global\RSC@fltrue}
23 \DeclareOption{captionleft}{\global\RSC@cltrue}
24 \DeclareOption{cl}{\global\RSC@cltrue}
25 \DeclareOption{chapter}{\global\RSC@chaptertrue}
26 \PassOptionsToPackage{chapter}{chemscheme}
27 \DeclareOption{ch}{\global\RSC@chaptertrue}
28 \PassOptionsToPackage{chapter}{chemscheme}
29 \DeclareOption{angew}{\global\RSC@angewtrue}
30 \global\RSC@cltrue}
31 \DeclareOption{natbib}{\global\RSC@natbibtrue}
32 \DeclareOption{chemcompounds}%
33 {\PassOptionsToPackage{chemcompounds}{chemscheme}}
34 \ProcessOptions
```

The `chemscheme` package is loaded to provide scheme environment. It is loaded here to ensure the options are correct.

```
35 \RequirePackage{chemscheme}
```

The choice of `natbib` or `cite` is then handled.

```
36 \ifRSC@natbib
37   \RequirePackage[numbers,sort&compress,super]{natbib}
38 \else
39   \RequirePackage[super]{cite}
40 \fi
```

8.2 Extra units and related commands

A few additional unit types are provided, which the `unitsdef` package omits for some reason.

```
\cubiccentimeter
\cmc 41 \newunit{\cubiccentimeter}{\cm\unitsuperscript{3}}
\Hz 42 \newcommand*{\cmc}{\cubiccentimeter}
\Molar 43 \newcommand*{\Hz}{\hertz}
\molar 44 \newunit{\Molar}{\textsc{m}}
mmHg 45 \newunit{\molar}{\mole\unitsep\dm\unitsuperscript{--3}}
46 \newunit{\mmHg}{mm\unitsep{}Hg}
```

In a very similar vein, the “standard state” symbol is handy. This is produced by rotating a symbol from the AMS set. Note that the rotation angle here has been carefully checked, but is set by eye!

```
\standardstate
47 \newcommand*{\standardstate}%
48   {\textsuperscript{\rotatebox[origin=c]{140.8}%
49     {\ensuremath{\varnothing}}}}
```

8.3 Alkyl radicals

Next we provide alkyl radical symbols, in a convenient form. The format depends on the journal asked for.

```
\iPr
\iBu 50 \newcommand*{\iPr}%
\sBu 51   {\ifRSC@angew\emph{i}Pr\else Pr\textsuperscript{i}\fi}
\tBu 52 \newcommand*{\iBu}%
53   {\ifRSC@angew\emph{i}Bu\else Bu\textsuperscript{i}\fi}
54 \newcommand*{\sBu}%
55   {\ifRSC@angew\emph{s}Bu\else Bu\textsuperscript{s}\fi}
56 \newcommand*{\tBu}%
57   {\ifRSC@angew\emph{t}Bu\else Bu\textsuperscript{t}\fi}
```

8.4 Citation formatting

If the `angew` option is set, we have to format the citations correctly. The formatting commands depend on whether we're using `cite` or `natbib`. The format of the bibliography labels is also altered here.

```
58 \ifRSC@angew
59   \ifRSC@natbib
60     \renewcommand\NAT@open{[]\renewcommand\NAT@close{}}
61   \else
62     \def\@citess#1{\textsuperscript{[#1]}}
63   \fi
64   \else
65     \def\@biblabel#1{#1}
66 \fi
```

8.5 Caption and float formatting

The `caption` package is used to control the appearance of float captions. The macros provided by the `memoir` class do not allow sufficient control, and so the functions provided by `memoir` are ignored. `caption` is loaded with the correct default format for almost all floats. In the case of *Angew. Chem.* style formatting, tables are treated differently.

```
67 \ifRSC@angew
68   \RequirePackage[labelsep=period,labelfont=bf]{caption}
69   \captionsetup[table]{labelsep=colon}
70 \else
71   \RequirePackage[labelsep=quad,labelfont=bf]{caption}
72 \fi
```

By default, short (one line) captions are centred. Longer captions are typeset as paragraphs. To set all captions flush left, the `caption` package is instructed not to check for single line captions.

```
73 \ifRSC@cl
74   \captionsetup[singlelinecheck=off]
75 \else
76 \fi
```

In RSC journals, figures are referred to as “Fig.” rather than “Figure.” This is sorted out here.

```
77 \ifRSC@angew
78 \else
79   \renewcommand{\figurename}{Fig.}
80 \fi
```

The next step is to format the floats themselves correctly. Unfortunately, `memoir` does not provide all of the commands needed to achieve this. Thus the `float` package is needed; in order to load it, the `\newfloat` command in `memoir` is killed off. Notice that if `memoir` is not in use, the `chemscheme` package will have already loaded `float`.


```

81 \@ifclassloaded{memoir}
82   {\let\newfloat\@undefined
83    \RequirePackage{float}}
84   {}

```

The standard float types are now restyled to place the captions correctly. The placement of captions is also altered so that they default to “here” if possible.

```

85 \floatstyle{plaintop}
86 \restylefloat{table}
87 \floatstyle{plain}
88 \restylefloat{scheme}
89 \restylefloat{figure}
90 \floatplacement{table}{htbp}
91 \floatplacement{scheme}{htbp}
92 \floatplacement{figure}{htbp}

```

The centring of floats is sorted out here, using macros provided by the `chemescheme` package.

```

93 \ifRSC@fl
94   \floatcontentsleft
95 \else
96   \floatcontentscentre
97 \fi

```

Finally, the naming for cross-references is sorted out properly, using the `varioref` package.

```

98 \labelformat{scheme}{\schemename~#1}
99 \labelformat{figure}{\figurename~#1}
100 \labelformat{table}{\tablename~#1}

```

9 The BibTeX style files

A great deal of the BibTeX style file information is lifted more or less directly from the standard style files, the `custom-bib` package or *Taming the Beast*. The rest consists of minor edits to obtain the correct format or support the `natbib` and `mcite` packages. Only two functions are novel to this package, and are given here for the interested reader.

The `strip.comma` function is used to “unwind” the comma added by `output.nonnull`, so that editors in brackets are easy to do. This is needed for the `angew` option.

```

101 FUNCTION {strip.comma}
102 { duplicate$
103   string.length 'find_length :=
104   duplicate$
105   find_length #1 - #1 substring$
106   ", " =
107     { #1 find_length #2 - substring$
108       " " *
109     }

```

```

110     'skip$
111   if$
112 }
113

```

`n.separate` is given in the `custom-bib` package. The following function is modified to separate out a number of any length into digit groups, *e.g.* 12345 turns into 12 345, 1234567 in 1 234 567 but 1234 or a12345 are left alone.

```

114 FUNCTION {n.separate.multi}
115 { 't :=
116   ""
117   #0 'numnames :=
118   t text.length$ #4 > t is.a.number and
119   {
120     { t empty$ not }
121     { t #-1 #1 substring$ is.a.number
122       { numnames #1 + 'numnames := }
123       { #0 'numnames := }
124       if$
125       t #-1 #1 substring$ swap$ *
126       t #-2 global.max$ substring$ 't :=
127       numnames #4 =
128       { duplicate$ #1 #1 substring$ swap$
129         #2 global.max$ substring$
130         "\," swap$ * *
131         #1 'numnames :=
132       }
133       'skip$
134       if$
135     }
136     while$
137   }
138   { t swap$ * }
139   if$
140 }
141

```

Change History

v1.0	support	1
General: Initial release of packaged	General tidying of code	1
rsc.bst	1	v2.1
v2.0	General: Moved float centring to	
General: Complete re-write of float	chemscheme package	1

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Numbers written in *italic* refer to the page where the corresponding entry is described; numbers underlined refer to the code line of the definition; numbers in *roman* refer to the code lines where the entry is used.

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