LaTeX for chemists: filling in the gaps

Joseph Wright

August 2, 2009

Abstract

LaTeX is traditionally strongly favoured by mathematicians and physicists. Use by chemists has tended to remain on the 'physical' side of the subject. Support for the particular needs of chemists has therefore be somewhat variable. I have been involved with a selection of new or improved packages, which seek to address some of the gaps.

1 Introduction

LaTeX has a whole range of packages available, aimed at almost the entire range of (academic) pursuits. However, gaps still arise, and are filled by interested users. For chemists, despite the existence of some very useful tools, gaps have remained. As I have worked with LaTeX, I have worked to fill some of those gaps, as far as I have been able. This article gives an overview of the areas I have contributed to, as well as highlights from others, and showing some gaps that remain. All of my packages are available from CTAN in the usual manner: to keep the bibliography a little shorter, these are not formally cited although other people's packages are.

Some chemistry-focussed packages will be mentioned in the rest of this article. However, one which deserves particular mention here is mhchem.[1] This allows very simple input of chemical formulae (and simple in-line equations). Thus, it allows you to write `\ce{H2SO4}` to get H_2SO_4, `\ce{CH2=CH-C#CH}` to get $CH_2{=}CH{-}C{\equiv}CH$, or

```
\ce{2H2 + O2 -> 2H2O}
```

and get

$$2\,H_2 + O_2 \longrightarrow 2\,H_2O. \tag{1}$$

It is a tool no chemist using LaTeX should be without.

2 Bibliography tools

2.1 BibTeX styles

One area where chemists seem to have unusual requirements is in creating bibliographies. To begin with, as a chemist the name is wrong: it is the *References*

section. The most basic requirement for everyone using BibTeX is appropriate style files. When I started using LaTeX, I found the `pccp.bst` BibTeX style, based on the journal *Physical Chemistry Chemical Physics*. However, there were problems with the output. I therefore wrote my own style, `rsc.bst`, based on the general requirements of the Royal Society of Chemistry (RSC); as a U.K.-based worker, the RSC style is one I follow for my own documents. Over time, `rsc.bst` was joined by `angew.bst`, aiming at the requirements of *Angewandte Chemie* (arguably the 'top' general chemistry journal: I'm sure a lot of American chemists would disagree!). These files, plus some utility macros, ended up in a package called rsc. Later, the utility macros moved elsewhere, but the rsc survives in modified form.

The achemso package was originally written by Mats Dahlgren, and provided a BibTeX style following the requirements of the American Chemical Society (ACS). Once I started using the style, I spotted some issues. Contacting the author, I found he no longer had time for package maintenance. So, as much by accident as by design, I took over achemso. A complete re-write resulted, with improvement to the BibTeX style and the accompanying LaTeX package. More recently, I've re-written the package again so that it fits in with the submission system at the ACS: this hopefully makes submitting articles a bit easier.

2.2 Bibliography packages

Beyond BibTeX styles, chemists have two important requirements for bibliographies. First, the idea of 'compound' references is common. Most chemistry journals use numerical citations, rather than the author–date system. It is very common to want a single reference number to refer to several related journal articles. The mcite package[2] can do this, but with very limited control of the results. In particular, it s common in chemistry to give each reference a letter inside a long list, such as

> [4] (*a*) G. Alberti, M. Casciola, U. Costantino, A. Peraio and E. Montoneri, *Solid State Ionics*, 1992, **50**, 315–322; (*b*) G. Alberti, M. Casciola, U. Costantino and R. Vivani, ...

The mcite package cannot do this automatically. So I began to consider the issue, and to ask on `comp.text.tex` if anyone had contact details for the author of mcite. Luckily, Michael Shell was interested in the other extensions to mcite: the result was the mciteplus package,[3] which *can* generate the desired output with control of formatting. Although I did not write any of mciteplus, the aim of making sub-lists inside each reference is included there specifically because I worked with him to get it working. Thus the example citation above can be given in the source simply as

```
\cite{Alberti1992,*Alberti1996}
```

which results in nicely-formatted output.[4] This document uses my `rsc.bst` BibTeX style, which sets up mciteplus to follow the requirements of the RSC;

for example, this instructs mciteplus to use a sub-list, and to make the sub-labels italic.

The second thing that chemists like to do is mix notes and references. This can be done by creating a BibTeX database of notes for every document you write to contain the information, but it is tedious. A much better idea would be to add the text directly into the body of the file, and have it move automatically to the bibliography section. To achieve this, I wrote the notes2bib package. The package works by creating a database for the notes during the LaTeX run, and then ensuring it is added to the list of files to be processed by BibTeX. This means it is 'neutral' with respect to sorting of bibliographies and packages used, such as cite,[5] natbib,[6] biblatex,[7] *etc*. Using notes2bib implies using numerical citations: the citations do not make much sense with the author–year system! Using the package requires only inclusion of one or more `\bibnote`s in the source, although it is possible to convert `\footnote` or `\endnote` entries into `\bibnote` data automatically. For example, you could write

```
\bibnote{An example bibliographic note}
```

and this would give.[8]

3 Utilities

The mhchem package is probably the most useful general utility package for chemists. However, this leaves a few gaps that can happily be filled. Initially, I provided a package with the rsc bundle to do this. However, later it became clear there was a better approach. The chemstyle package inherited the utilities from rsc, along with new functions. For example, this gives the macros `\tBu`, `\iPr`, *etc*. to give alkyl radicals: *t*-Bu, *i*-Pr, *etc*. It also provides items such as the 'standard state' symbol, to allow you to produce $\Delta H^\ominus$ easily.

The main aim of chemstyle is to help maintain consistency. By specifying the journal style to follow, the package allows float captions, cross-referencing and so on to follow the choices of the publication given. This is a lot easier than trying to remember the choices of every separate journal. It also loads a number of useful packages for the chemist, including my own chemscheme.

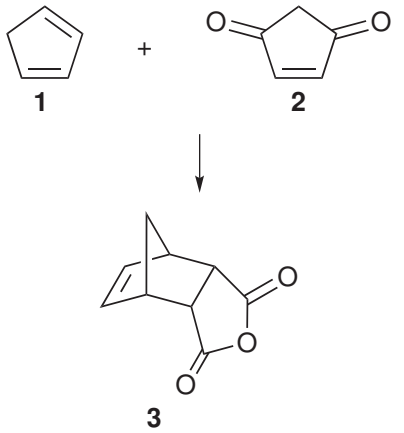
4 Graphics: the 'scheme'

The concept of a 'scheme' is one that non-chemists find difficult to understand: they expect the name 'equation' to be used. An equation to most synthetic chemists is a simple, broadly non-graphical item, such as Equation 2.

$$2\,H_2 + O_2 \longrightarrow 2\,H_2O \tag{2}$$

In contrast, a scheme is a more complex, graphically-rich item, such as Scheme 1. The example here is simple by the standards of many schemes in the research literature. Several packages are available for generating the graphics directly in

LaTeX. However, producing anything beyond the most simple scheme becomes very difficult using text-based tools. I, like almost every synthetic chemist, use the commercial package ChemDraw[9] to produce my schemes.



Scheme 1: A simple scheme

Rather than trying to provide a package to tackle directly producing schemes in LaTeX, the chemscheme package aims to solve two lesser problems. The first aim of chemscheme is to provide an 'out of the box' float for schemes. Chemists expect the scheme to be near 'here' if possible, so this is the case with the `scheme` float. Thus the example scheme used here is produced using

```
\begin{scheme}
  \includegraphics{Scheme}
  \caption{A simple scheme}
  \label{sch}
\end{scheme}
```

The second aim is more complex. The use of reference numbers for chemicals in graphics is very common. Two packages exist to automate this in the text: bpchem[10] and chemcompounds.[11] However, neither can work with graphical content. Using PSfrag,[12] the chemscheme package makes automatic substitution easy for `.eps` graphics. This is achieved by the `\schemeref` macro, which works with a temporary marker in the input. By using pst-pdf[13] this can also be used with PDFLaTeX.

5 biblatex bibliographies

The biblatex, currently available with beta status, is a completely new way to produce bibliographies from a database. The current version uses BibTeX, but does not need dedicated style files to do this. Instead, it requires LaTeX files

containing formatting instructions. I've written some of these for chemists and other scientists: biblatex-chem to cover the same journals as rsc and achemso, biblatex-nature for *Nature*-like formatting and biblatex-science to emulate the journal *Science*.

6 Further afield

Beyond the focus on chemistry, one package in particular deserves mention here. Using units with numbers is common across the whole of science. The siunitx package provides a wide range of tools for typing units and values. For example, the input

```
$R = \SI[dp=3]{8.314472}
  {\joule\per\mole\per\kelvin}$
```

gives the typeset result $R = 8.314\,\mathrm{J\,mol^{-1}\,K^{-1}}$, while

```
$R = \SI[dp=5,per=slash]{8.314472}
  {\joule\per\mole\per\kelvin}$
```

gives $R = 8.314\,47\,\mathrm{J/(mol\,K)}$. This type of format control is available either on a per-macro basis or by setting package settings in the document. The aim of siunitx is therefore to allow units and values to have a single input syntax but give a range of output formats: this makes working with different publishing requirements much easier.

References

[1] M. Hensel, *The mhchem Bundle*, Available from CTAN, `macros/latex/contrib/mhchem`, 2007.

[2] T. Ohl, *mcite: Multiple Citations on One Key*, Available from CTAN, `macros/latex/contrib/mcite`, 2005.

[3] M. Shell, *Mciteplus: Enhanced Multicitations*, Available from CTAN, `macros/latex/contrib/mciteplus`, 2008.

[4] (*a*) G. Alberti, M. Casciola, U. Costantino, A. Peraio and E. Montoneri, *Solid State Ionics*, 1992, **50**, 315–322; (*b*) G. Alberti, M. Casciola, U. Costantino and R. Vivani, *Adv. Mater.*, 1996, **8**, 291–303.

[5] D. Arseneau, *cite*, Available from CTAN, `macros/latex/contrib/cite`, 2009.

[6] P. W. Daly, *Natural Sciences Citations and References*, Available from CTAN, `macros/latex/contrib/natbib`, 2009.

[7] P. Lehman, *The biblatex package*, Available from CTAN, `macros/latex/exptl/biblatex`, 2009.

[8] An example bibliographic note.

[9] See `http://www.cambridgesoft.com`.

[10] B. Pedersen, *The bpchem package*, Available from CTAN, `macros/latex/contrib/bpchem`, 2004.

[11] S. Schenk, *The chemcopounds package*, Available from CTAN, `macros/latex/contrib/chemcompounds`, 2006.

[12] M. C. Grant and D. Carlisle, *The PSfrag system, version 3*, Available from CTAN, `macros/latex/contrib/psfrag`, 1998.

[13] R. Nieprashk and H. Gäßlein, *The pst-pdf package*, Available from CTAN, `macros/latex/contrib/pst-pdf`, 2008.