chemsym – a LaTeX Macro for Chemical Symbols*

Mats Dahlgren†

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Abstract

This document describes the chemsym package, which makes it easier to type chemical symbols correctly, without having to worry about math mode or text mode. Furthermore, chemsym makes both the super- and the subscript commands (`^` and `_`) and '·' (`\cdot`) available in text mode.

1 Introduction

chemsym is a LaTeX package which makes it easier to type chemical symbols correctly. It defines a command for each element of the periodic table (the 109 first), Deuterium, the Methyl, Ethyl and Butyl groups[1] (for the Propyle group, use `\Pr`, Praseodymium), and the −OH, −COOH, and −CH groups.[2] The use of the commands results in a up-right chemical symbol, regardless of whether it is used in math mode or text mode. If not followed by a sub- or superscript, a `(`, a `)`, a `[`, or a `]` a small space is added (slightly less than what '`\,`' gives).

In late 1997, IUPAC (International Union of Pure and Applied Chemistry) issued new recommendations for the names and symbols for elements 104-109 ("Names and symbols of transfermium elements (IUPAC recommendations 1997)", *Pure and Applied Chemistry* **1997**, *69*(12), 2471-2473). The recommended names are Rutherfordium, Rf, Dubnium, Db, Seaborgium Sg, Bohrium, Bh, Hassnium, Hs, and Meitnerium, Mt, respectively. From the previous recommendations in 1994, all but Bh and Mt have changed.

This userguide is also available in `.pdf`-format on the internet. It is found from my LaTeX web page: `http://www.homenet.se/matsd/latex/`

2 Userguide

2.1 Requirements

The file `chemsym.sty` must be available in the user's `TEXINPUTS` directories. It requires LaTeX 2_ε of 1996/12/01 (or newer).

*This document describes chemsym version 2.0, and was last updated 1998/06/24.

†Email: `matsd@sssk.se` Web: `http://www.homenet.se/matsd/`

[1] Suggested by Ulf Henriksson (`ulf@physchem.kth.se`).

[2] Suggested in part by Axel Kielhorn (`i0080108@ws.rz.tu-bs.de`)

2.2 Usage

The package is included by stating

`\usepackage[`*option*`]{chemsym}`

In the document preamble. The only option which has any effect on chemsym is `collision`, see below.

2.3 Commands

chemical symbols

The chemsym package defines 116 user commands; one for each of the 109 first elements, Deuterium, the Methyl, Ethyl and Butyl groups (for the Propyle group, use `\Pr`, Praseodymium), and the −OH, −COOH, and −CH groups. The command names are all made up of the chemical symbol preceeded by '\'; thus for Nitrogen, N, you type `\N`, and for Mercury, Hg, `\Hg`, etc. These commands appear to be robust. To obtain 'CH_2', you simply type '`\CH_2`' in your input file; 'CH_3' is obtained by typing '`\CH_3`' (of course).

\H \O \P \S \Re \Pr Sb

Since there are six commands in TEX/LATEX already of this kind (`\H`, `\O`, `\P`, `\S`, `\Re`, and `\Pr`), and one environment in $\mathcal{AMS}$-LATEX (the `Sb` environment),[3] these old commands have to be renamed. The names of choice are shown in the table below.

TEX command	With chemsym you write	Use/Example
`\H`	`\h`	The accent in 'ő'
`\O`	`\OO`	Ø
`\P`	`\PP`	¶
`\S`	`\Ss`	§
`\Re`	`\re`	$\Re$ (in math mode)
`\Pr`	`\pr`	Pr (in math mode)
`\begin{Sb}`	`\begin{SB}`	(with $\mathcal{AMS}$-LATEX)
`\end{Sb}`	`\end{SB}`	(with $\mathcal{AMS}$-LATEX)

\kemtkn \nsrrm \nsrrms ^ _

Also, `\kemtkn`, a command for defining other chemical symbols and similar functions is available. `\kemtkn` takes one mandatory argument (the string to treat as a chemical symbol). Two other internal commands, `\nsrrm` and `\nsrrms` are also available. `\nsrrm` simply puts its (mandatory) argument in `mathrm`. `\nsrrms` does the same, but also adds a small space after it. This space is a second, optional, argument to `\nsrrms` which should be given in `em` units (without '`em`'). The default is `0.1em`. For convenience when typing chemical formulas and units with exponents, the super- and subscript commands `^` and `_` are made available also outside of math mode, provided the option `collision` is *not* specified. Thus, with chemsym you can type `m^2` instead of `m$^2$` for m^2 also in text mode. Analogously, you can type `\H_2\O` for H_2O in both math and text mode and get the same result. Notice that text which you may put in the arguments of `^` and `_` automatically is set in math mode. So if you want 'M_q' you must type `M_{\mathrm{q}}` and not only `M_q`, the latter comes out as 'M_q'. (This feature is not seriously disturbing since this feature with `^` and `_` is intended to be used mainly with numbers in the arguments.)

\cdot

Futhermore, the `\cdot` command (producing a '·') is also available outside math mode. This feature is included to facilitate typing formulas like "$CH_3 \cdot CH_3$" (`\CH_3\cdot\CH_3`) also in text mode.[4]

[3] Thanks to Thorsten Löhl (`lohl@uni-muenster.de`) for pointing out this.

[4] Also suggested by Ulf Henriksson (`ulf@physchem.kth.se`).

2.4 The `collision` option

`collision` To avoid probelms with other packages due to `^` (and `_`) being active, this may be swithced off by stating the option `collision` when loading the chemsym package. If you get the following error message (or a similar), you are likely to have such a collision with chemsym involved (in this case with longtable):

```
! Argument of ^ has an extra }.
<inserted text>
                \par
l.120 \end{longtable}

?
```

To solve the problem, state the `collision` option *and* delete the `.aux` file before running LaTeX again. Some packages contain `^^J`-constructs which may not always be apparent to the user. One example, which collides with chemsym, is the multicol package's warning if you specify only one column. In that case, the error message is:

```
! Argument of ^ has an extra }.
<inserted text>
                \par
l.18 \begin{multicols}{1}

?
```

In this case, you *may* come around the problem by specifying a number of columns ≥ 2; if not, specify the `collision` option for the chemsym package.

3 Examples

This section gives some simple examples of the use of chemsym. To write the formula for water in both math and text mode, you type `\H_2\O{}`, which gives H_2O as result. Notice that this differs from typing `\H$_2$\O`, which gives H_2O as result. In the first example, there is not any extra space added after the H. This addition of space makes formulas like HCN (`\H\C\N`) easier to read than just typing `HCN`: HCN.

The use of the commands of chemsym is specially useful when chemical symbols are used as indices in equations. The following example illustrates this:

$$\mathcal{M}_{\mathrm{Fe(H_2O)_6}} = 6\mathcal{M}_{\mathrm{H_2O}} + \mathcal{M}_{\mathrm{Fe}} \tag{1}$$

which was obtained by typing

```
\begin{equation}
\mathcal{M}_{\Fe(\H_2\O)_6} = 6\mathcal{M}_{\H_2\O} + \mathcal{M}_{\Fe}
\end{equation}
```

It is also easy to define other chemical symbols commands, such as commands for specific isotopes. Suppose you rather want to use the notation ^{2}H than D for Deuterium. This may be defined as:

```
\newcommand{\hH}{\kemtkn{{}^2H}}
```

(which was used above: `...notation \hH{} than \D{} for...`). Internally, chemsym uses a syntax like this to def ine the various commands for the chemical symbols.[5]

After running `chemsym.ins` through LaTeX 2ε, you can typeset the Periodic Table of the Elements by running LaTeX 2ε on the file `pertab.tex`. (It fits fine on an A4 paper, and there should be no problem with a U.S. lettersize paper as well.) The Periodic Table requires the rotating package, which in turn requires the packages graphicx and ifthen.

4 Known Problems

- Since chemsym makes `^` and `_` active, it will collide with other packages which make use of constructs like `^^J` (*e. g.* the longtable package). To avoid this problem, specify the option `collision` when loading chemsym (or globally).
- If the chemsym package is used together with the rotating or amstex package, chemsym should be loaded last.
- If the chemsym package is used together with the fancyheadings package, fancyheadings should be loaded after chemsym.[6]
- Since chemsym makes `_` and `^` active, these characters cannot be used in labels when using the chemsym package, nor in file names loaded in LaTeX runs loading the chemsym package (unless you specify the `collision` option).[7]
- Also since `^` is made active, when following after a prime in math mode (`'`), a "double superscript" error is produced unless a double bracing (`{}`) is included before the `^` character.[8] Thus, you should type `x'{}^2` instead of `x'^2` when using chemsym to obtain x'^2.

5 Sending a Bug Report

chemsym is likely to contain bugs, and reports about them are most welcome. Before filing a bug report, please take the following actions:

1. Ensure your problem is not due to your own input file, package(s), or class(es);
2. Ensure your problem is not covered in the section "Known Problems" above;
3. Try to locate the problem by writing a minimal LaTeX input file which reproduces the problem. Include the command
   `\setcounter{errorcontextlines}{999}`
   in your input;
4. Run your file through LaTeX;
5. Send a description of your problem, the input file and the log file via e-mail to:
   `matsd@sssk.se`.

Enjoy your LaTeX!

mats d.

[5] To make the command robust, say `\newcommand{\hH}{\protect\kemtkn{{}}^2H}}` or use the command `\DeclareRobustCommand` instead of `\newcommand`.

[6] Thanks to Lars Reinton (`larsr@stud.unit.no`) for pointing out this.

[7] Thanks to Axel Kielhorn (`i0080108@ws.rz.tu-bs.de`) for pointing out this problem.

[8] Thanks to Jeroen Paasschens (`paassche@natlab.research.philips.com`) for bringing my attention to this problem.

6 The Code

For the interested reader(s), here is a short description of the code. First, the package is to identify itself:

```
\NeedsTeXFormat{LaTeX2e}[1996/12/01]
\ProvidesPackage{chemsym}[1998/05/31 v.2.0 Chemical symbols]
```

First in the real code, we have to rename the old functions `\H`, `\O`, `\P`, `\S`, `\Re`, and `\Pr`:

```
\let\h=\H
\let\OO=\O
\let\PP=\P
\let\Ss=\S
\let\re=\Re
\let\pr=\Pr
```

Here we check if the $\mathcal{AMS}$-LaTeX package is loaded, and if so, change the `Sb` environment to be called `SB`.

```
\@ifundefined{Sb}{\def\Sb{\protect\kemtkn{Sb}}}%
  {\let\SB=\Sb \let\endSB=\endSb}
```

Now, we make `^`, `_`, and `\cdot` work without `$...$` also in text mode – if not switched off. To do this, we need a boolean and some option processing...

```
\newif  \ifc@llsn  \c@llsnfalse
\DeclareOption{collision}{\global\c@llsntrue}
\DeclareOption*{\OptionNotUsed}
\ProcessOptions*
\ifc@llsn\AtEndDocument{%
  \PackageWarningNoLine{chemsym}{Due to possible collisions with other
  \MessageBreak packages, super- and subscrips are not avaliable
  \MessageBreak outside math mode despite your loading of `chemsym'}}
\else
  \def\sprscrpt#1{\ensuremath{^{#1}}}
  \def\sbscrpt#1{\ensuremath{_{#1}}}
  \catcode`\^ \active
  \catcode`\_ \active
  \let^=\sprscrpt
  \let_=\sbscrpt
\fi
\@ifundefined{cd@t}{%
\let\cd@t=\cdot
\def\cdot{\ensuremath{\cd@t}}}{}
```

(The `\@ifundefined` is required for local compatibility reasons at my former site.) Then, some general macros are defined:

```
\newcommand{\nsrrm}[1]{\ensuremath{\mathrm{#1}}}
\newcommand{\nsrrms}[2][0.1]{\ensuremath{\mathrm{#2}\kern #1em}}
\newcommand{\kemtkn}[1]{\@ifnextchar_{\nsrrm{#1}}{\@ifnextchar^{\nsrrm{#1}}%
  {\@ifnextchar){\nsrrm{#1}}{\@ifnextchar({\nsrrm{#1}}%
  {\@ifnextchar]{\nsrrm{#1}}{\@ifnextchar[{\nsrrm{#1}}{\nsrrms{#1}}}}}}}}
```

As you can see, you can change the spacing in the chemical formulas by making changes to `\nsrrms`. This you can do with `\renewcommand` in your document preamble or in another package file. Then we define the 110 commands for chemical symbols:

```
\renewcommand{\H}{\protect\kemtkn{H}} % modified
\newcommand{\D}{\protect\kemtkn{D}}
```

```
\newcommand{\He}{\protect\kemtkn{He}}
\newcommand{\Li}{\protect\kemtkn{Li}}
\newcommand{\Be}{\protect\kemtkn{Be}}
\newcommand{\B}{\protect\kemtkn{B}}
\newcommand{\C}{\protect\kemtkn{C}}
\newcommand{\N}{\protect\kemtkn{N}}
\renewcommand{\O}{\protect\kemtkn{O}} % modified
\newcommand{\F}{\protect\kemtkn{F}}
\newcommand{\Ne}{\protect\kemtkn{Ne}}
\newcommand{\Na}{\protect\kemtkn{Na}}
\newcommand{\Mg}{\protect\kemtkn{Mg}}
\newcommand{\Al}{\protect\kemtkn{Al}}
\newcommand{\Si}{\protect\kemtkn{Si}}
\renewcommand{\P}{\protect\kemtkn{P}} % modified
\renewcommand{\S}{\protect\kemtkn{S}} % modified
\newcommand{\Cl}{\protect\kemtkn{Cl}}
\newcommand{\Ar}{\protect\kemtkn{Ar}}
\newcommand{\K}{\protect\kemtkn{K}}
\newcommand{\Ca}{\protect\kemtkn{Ca}}
\newcommand{\Sc}{\protect\kemtkn{Sc}}
\newcommand{\Ti}{\protect\kemtkn{Ti}}
\newcommand{\V}{\protect\kemtkn{V}}
\newcommand{\Cr}{\protect\kemtkn{Cr}}
\newcommand{\Mn}{\protect\kemtkn{Mn}}
\newcommand{\Fe}{\protect\kemtkn{Fe}}
\newcommand{\Co}{\protect\kemtkn{Co}}
\newcommand{\Ni}{\protect\kemtkn{Ni}}
\newcommand{\Cu}{\protect\kemtkn{Cu}}
\newcommand{\Zn}{\protect\kemtkn{Zn}}
\newcommand{\Ga}{\protect\kemtkn{Ga}}
\newcommand{\Ge}{\protect\kemtkn{Ge}}
\newcommand{\As}{\protect\kemtkn{As}}
\newcommand{\Se}{\protect\kemtkn{Se}}
\newcommand{\Br}{\protect\kemtkn{Br}}
\newcommand{\Kr}{\protect\kemtkn{Kr}}
\newcommand{\Rb}{\protect\kemtkn{Rb}}
\newcommand{\Sr}{\protect\kemtkn{Sr}}
\newcommand{\Y}{\protect\kemtkn{Y}}
\newcommand{\Zr}{\protect\kemtkn{Zr}}
\newcommand{\Nb}{\protect\kemtkn{Nb}}
\newcommand{\Mo}{\protect\kemtkn{Mo}}
\newcommand{\Tc}{\protect\kemtkn{Tc}}
\newcommand{\Ru}{\protect\kemtkn{Ru}}
\newcommand{\Rh}{\protect\kemtkn{Rh}}
\newcommand{\Pd}{\protect\kemtkn{Pd}}
\newcommand{\Ag}{\protect\kemtkn{Ag}}
\newcommand{\Cd}{\protect\kemtkn{Cd}}
\newcommand{\In}{\protect\kemtkn{In}}
\newcommand{\Sn}{\protect\kemtkn{Sn}}
\renewcommand{\Sb}{\protect\kemtkn{Sb}}  % modified with AMS-LaTeX
\newcommand{\Te}{\protect\kemtkn{Te}}
\newcommand{\I}{\protect\kemtkn{I}}
\newcommand{\Xe}{\protect\kemtkn{Xe}}
\newcommand{\Cs}{\protect\kemtkn{Cs}}
```

```
\newcommand{\Ba}{\protect\kemtkn{Ba}}
\newcommand{\La}{\protect\kemtkn{La}}
\newcommand{\Ce}{\protect\kemtkn{Ce}}
\renewcommand{\Pr}{\protect\kemtkn{Pr}} % modified
\newcommand{\Nd}{\protect\kemtkn{Nd}}
\newcommand{\Pm}{\protect\kemtkn{Pm}}
\newcommand{\Sm}{\protect\kemtkn{Sm}}
\newcommand{\Eu}{\protect\kemtkn{Eu}}
\newcommand{\Gd}{\protect\kemtkn{Gd}}
\newcommand{\Tb}{\protect\kemtkn{Tb}}
\newcommand{\Dy}{\protect\kemtkn{Dy}}
\newcommand{\Ho}{\protect\kemtkn{Ho}}
\newcommand{\Er}{\protect\kemtkn{Er}}
\newcommand{\Tm}{\protect\kemtkn{Tm}}
\newcommand{\Yb}{\protect\kemtkn{Yb}}
\newcommand{\Lu}{\protect\kemtkn{Lu}}
\newcommand{\Hf}{\protect\kemtkn{Hf}}
\newcommand{\Ta}{\protect\kemtkn{Ta}}
\newcommand{\W}{\protect\kemtkn{W}}
\renewcommand{\Re}{\protect\kemtkn{Re}} % modified
\newcommand{\Os}{\protect\kemtkn{Os}}
\newcommand{\Ir}{\protect\kemtkn{Ir}}
\newcommand{\Pt}{\protect\kemtkn{Pt}}
\newcommand{\Au}{\protect\kemtkn{Au}}
\newcommand{\Hg}{\protect\kemtkn{Hg}}
\newcommand{\Tl}{\protect\kemtkn{Tl}}
\newcommand{\Pb}{\protect\kemtkn{Pb}}
\newcommand{\Bi}{\protect\kemtkn{Bi}}
\newcommand{\Po}{\protect\kemtkn{Po}}
\newcommand{\At}{\protect\kemtkn{At}}
\newcommand{\Rn}{\protect\kemtkn{Rn}}
\newcommand{\Fr}{\protect\kemtkn{Fr}}
\newcommand{\Ra}{\protect\kemtkn{Ra}}
\newcommand{\Ac}{\protect\kemtkn{Ac}}
\newcommand{\Th}{\protect\kemtkn{Th}}
\newcommand{\Pa}{\protect\kemtkn{Pa}}
\newcommand{\U}{\protect\kemtkn{U}}
\newcommand{\Np}{\protect\kemtkn{Np}}
\newcommand{\Pu}{\protect\kemtkn{Pu}}
\newcommand{\Am}{\protect\kemtkn{Am}}
\newcommand{\Cm}{\protect\kemtkn{Cm}}
\newcommand{\Bk}{\protect\kemtkn{Bk}}
\newcommand{\Cf}{\protect\kemtkn{Cf}}
\newcommand{\Es}{\protect\kemtkn{Es}}
\newcommand{\Fm}{\protect\kemtkn{Fm}}
\newcommand{\Md}{\protect\kemtkn{Md}}
\newcommand{\No}{\protect\kemtkn{No}}
\newcommand{\Lr}{\protect\kemtkn{Lr}}
\newcommand{\Rf}{\protect\kemtkn{Rf}}
\newcommand{\Db}{\protect\kemtkn{Db}}
\newcommand{\Sg}{\protect\kemtkn{Sg}}
\newcommand{\Bh}{\protect\kemtkn{Bh}}
\newcommand{\Hs}{\protect\kemtkn{Hs}}
\newcommand{\Mt}{\protect\kemtkn{Mt}}
```

At last, we define the three alkyle groups and some other useful groups as chemical symbols:

```
\newcommand{\Me}{\protect\kemtkn{Me}}
\newcommand{\Et}{\protect\kemtkn{Et}}
\newcommand{\Bu}{\protect\kemtkn{Bu}}
\newcommand{\OH}{\protect\kemtkn{OH}}
\newcommand{\COOH}{\protect\kemtkn{COOH}}
\newcommand{\CH}{\protect\kemtkn{CH}}
```

This brings us to the end of chemsym. Hope you'll enjoy it!