

chemsym – a L^AT_EX Macro for Chemical Symbols*

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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.

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1 Introduction

`chemsym` is a L^AT_EX 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 groups¹ (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 Bhand Mt have changed.

This userguide is also available in .pdf-format on the internet. It is found from my L^AT_EX 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 L^AT_EX 2_ε of 1996/12/01 (or newer).

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

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

²Suggested 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 preceded 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` Since there are six commands in \TeX/\LaTeX already of this kind (`\H`, `\O`, `\P`, `\S`, `\Re`, and `\Pr`), and one environment in $\mathcal{AMS}\text{-}\LaTeX$ (the `Sb` environment),³ these old commands have to be renamed. The names of choice are shown in the table below.

`\S`
`\Re`
`\Pr`
`Sb`

| \TeX command | With chemsym you write | Use/Example |
|-------------------------|-------------------------|---------------------------------------|
| <code>\H</code> | <code>\h</code> | The accent in ‘ ó ’ |
| <code>\O</code> | <code>\OO</code> | \emptyset |
| <code>\P</code> | <code>\PP</code> | ¶ |
| <code>\S</code> | <code>\Ss</code> | § |
| <code>\Re</code> | <code>\re</code> | \Re (in math mode) |
| <code>\Pr</code> | <code>\pr</code> | Pr (in math mode) |
| <code>\begin{Sb}</code> | <code>\begin{SB}</code> | (with $\mathcal{AMS}\text{-}\LaTeX$) |
| <code>\end{Sb}</code> | <code>\end{SB}</code> | (with $\mathcal{AMS}\text{-}\LaTeX$) |

`\kemtkn` 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 `m2` 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` Furthermore, the `\cdot` command (producing a \cdot) 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

³Thanks to Thorsten Löhle (lohl@uni-muenster.de) for pointing out this.

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

2.4 The collision option

`collision` To avoid problems with other packages due to `^` (and `_`) being active, this may be switched 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
1.120 \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
1.18 \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:

$$\mathcal{M}_{\text{Fe}(\text{H}_2\text{O})_6} = 6\mathcal{M}_{\text{H}_2\text{O}} + \mathcal{M}_{\text{Fe}} \quad (1)$$

which was obtained by typing

```
\begin{equation}
\mathcal{M}_{\text{Fe}(\text{H}_2\text{O})_6} = 6\mathcal{M}_{\text{H}_2\text{O}} + \mathcal{M}_{\text{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 ^2H than `D` for Deuterium. This may be defined as:

```
\newcommand{\hH}{\kern-0.25ex\text{H}^2}
```

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

After running `chemsym.ins` through $\text{\LaTeX} 2_{\epsilon}$, you can typeset the Periodic Table of the Elements by running $\text{\LaTeX} 2_{\epsilon}$ 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.

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

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

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

⁸Thanks 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:

```
1 \NeedsTeXFormat{LaTeX2e}[1996/12/01]
2 \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`:

```
3 \let\h=\H
4 \let\O=\O
5 \let\PP=\P
6 \let\Ss=\S
7 \let\re=\Re
8 \let\pr=\Pr
```

Here we check if the *AMS-L^AT_EX* package is loaded, and if so, change the `Sb` environment to be called `SB`.

```
9 \@ifundefined{Sb}{\def\Sb{\protect\kern{Sb}}}%
10 {\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. . .

```
11 \newif \ifc@llsn \c@llsnfalse
12 \DeclareOption{collision}{\global\c@llsntrue}
13 \DeclareOption*{\OptionNotUsed}
14 \ProcessOptions*
15 \ifc@llsn\AtEndDocument{%
16   \PackageWarningNoLine{chemsym}{Due to possible collisions with other
17   \MessageBreak packages, super- and subscripts are not available
18   \MessageBreak outside math mode despite your loading of ‘chemsym’}}
19 \else
20   \def\sprscript#1{\ensuremath{^{\#1}}}
21   \def\sbscript#1{\ensuremath_{\#1}}
22   \catcode‘\^ \active
23   \catcode‘\_ \active
24   \let^=\sprscript
25   \let_=\sbscript
26 \fi
27 \@ifundefined{cd@t}{%
28 \let\cd@t=\cdot
29 \def\cdot{\ensuremath{\cd@t}}}{}
```

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

```
30 \newcommand{\nsrrm}[1]{\ensuremath{\mathrm{\#1}}}
31 \newcommand{\nsrrms}[2][0.1]{\ensuremath{\mathrm{\#2}\kern \#1em}}
32 \newcommand{\kernkern}[1]{\ifnextchar_{\nsrrm{\#1}}{\ifnextchar^{\nsrrm{\#1}}}%
33 {\@ifnextchar}{\nsrrm{\#1}}{\@ifnextchar({\nsrrm{\#1}}}%
34 {\@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:

```
35 \renewcommand{\H}{\protect\kern{H}} % modified
36 \newcommand{\D}{\protect\kern{D}}
```

```

37 \newcommand{\He}{\protect\kemtkn{He}}
38 \newcommand{\Li}{\protect\kemtkn{Li}}
39 \newcommand{\Be}{\protect\kemtkn{Be}}
40 \newcommand{\B}{\protect\kemtkn{B}}
41 \newcommand{\C}{\protect\kemtkn{C}}
42 \newcommand{\N}{\protect\kemtkn{N}}
43 \renewcommand{\O}{\protect\kemtkn{O}} % modified
44 \newcommand{\F}{\protect\kemtkn{F}}
45 \newcommand{\Ne}{\protect\kemtkn{Ne}}
46 \newcommand{\Na}{\protect\kemtkn{Na}}
47 \newcommand{\Mg}{\protect\kemtkn{Mg}}
48 \newcommand{\Al}{\protect\kemtkn{Al}}
49 \newcommand{\Si}{\protect\kemtkn{Si}}
50 \renewcommand{\P}{\protect\kemtkn{P}} % modified
51 \renewcommand{\S}{\protect\kemtkn{S}} % modified
52 \newcommand{\Cl}{\protect\kemtkn{Cl}}
53 \newcommand{\Ar}{\protect\kemtkn{Ar}}
54 \newcommand{\K}{\protect\kemtkn{K}}
55 \newcommand{\Ca}{\protect\kemtkn{Ca}}
56 \newcommand{\Sc}{\protect\kemtkn{Sc}}
57 \newcommand{\Ti}{\protect\kemtkn{Ti}}
58 \newcommand{\V}{\protect\kemtkn{V}}
59 \newcommand{\Cr}{\protect\kemtkn{Cr}}
60 \newcommand{\Mn}{\protect\kemtkn{Mn}}
61 \newcommand{\Fe}{\protect\kemtkn{Fe}}
62 \newcommand{\Co}{\protect\kemtkn{Co}}
63 \newcommand{\Ni}{\protect\kemtkn{Ni}}
64 \newcommand{\Cu}{\protect\kemtkn{Cu}}
65 \newcommand{\Zn}{\protect\kemtkn{Zn}}
66 \newcommand{\Ga}{\protect\kemtkn{Ga}}
67 \newcommand{\Ge}{\protect\kemtkn{Ge}}
68 \newcommand{\As}{\protect\kemtkn{As}}
69 \newcommand{\Se}{\protect\kemtkn{Se}}
70 \newcommand{\Br}{\protect\kemtkn{Br}}
71 \newcommand{\Kr}{\protect\kemtkn{Kr}}
72 \newcommand{\Rb}{\protect\kemtkn{Rb}}
73 \newcommand{\Sr}{\protect\kemtkn{Sr}}
74 \newcommand{\Y}{\protect\kemtkn{Y}}
75 \newcommand{\Zr}{\protect\kemtkn{Zr}}
76 \newcommand{\Nb}{\protect\kemtkn{Nb}}
77 \newcommand{\Mo}{\protect\kemtkn{Mo}}
78 \newcommand{\Tc}{\protect\kemtkn{Tc}}
79 \newcommand{\Ru}{\protect\kemtkn{Ru}}
80 \newcommand{\Rh}{\protect\kemtkn{Rh}}
81 \newcommand{\Pd}{\protect\kemtkn{Pd}}
82 \newcommand{\Ag}{\protect\kemtkn{Ag}}
83 \newcommand{\Cd}{\protect\kemtkn{Cd}}
84 \newcommand{\In}{\protect\kemtkn{In}}
85 \newcommand{\Sn}{\protect\kemtkn{Sn}}
86 \renewcommand{\Sb}{\protect\kemtkn{Sb}} % modified with AMS-LaTeX
87 \newcommand{\Te}{\protect\kemtkn{Te}}
88 \newcommand{\I}{\protect\kemtkn{I}}
89 \newcommand{\Xe}{\protect\kemtkn{Xe}}
90 \newcommand{\Cs}{\protect\kemtkn{Cs}}

```

```

91 \newcommand{\Ba}{\protect\kemtkn{Ba}}
92 \newcommand{\La}{\protect\kemtkn{La}}
93 \newcommand{\Ce}{\protect\kemtkn{Ce}}
94 \renewcommand{\Pr}{\protect\kemtkn{Pr}} % modified
95 \newcommand{\Nd}{\protect\kemtkn{Nd}}
96 \newcommand{\Pm}{\protect\kemtkn{Pm}}
97 \newcommand{\Sm}{\protect\kemtkn{Sm}}
98 \newcommand{\Eu}{\protect\kemtkn{Eu}}
99 \newcommand{\Gd}{\protect\kemtkn{Gd}}
100 \newcommand{\Tb}{\protect\kemtkn{Tb}}
101 \newcommand{\Dy}{\protect\kemtkn{Dy}}
102 \newcommand{\Ho}{\protect\kemtkn{Ho}}
103 \newcommand{\Er}{\protect\kemtkn{Er}}
104 \newcommand{\Tm}{\protect\kemtkn{Tm}}
105 \newcommand{\Yb}{\protect\kemtkn{Yb}}
106 \newcommand{\Lu}{\protect\kemtkn{Lu}}
107 \newcommand{\Hf}{\protect\kemtkn{Hf}}
108 \newcommand{\Ta}{\protect\kemtkn{Ta}}
109 \newcommand{\W}{\protect\kemtkn{W}}
110 \renewcommand{\Re}{\protect\kemtkn{Re}} % modified
111 \newcommand{\Os}{\protect\kemtkn{Os}}
112 \newcommand{\Ir}{\protect\kemtkn{Ir}}
113 \newcommand{\Pt}{\protect\kemtkn{Pt}}
114 \newcommand{\Au}{\protect\kemtkn{Au}}
115 \newcommand{\Hg}{\protect\kemtkn{Hg}}
116 \newcommand{\Tl}{\protect\kemtkn{Tl}}
117 \newcommand{\Pb}{\protect\kemtkn{Pb}}
118 \newcommand{\Bi}{\protect\kemtkn{Bi}}
119 \newcommand{\Po}{\protect\kemtkn{Po}}
120 \newcommand{\At}{\protect\kemtkn{At}}
121 \newcommand{\Rn}{\protect\kemtkn{Rn}}
122 \newcommand{\Fr}{\protect\kemtkn{Fr}}
123 \newcommand{\Ra}{\protect\kemtkn{Ra}}
124 \newcommand{\Ac}{\protect\kemtkn{Ac}}
125 \newcommand{\Th}{\protect\kemtkn{Th}}
126 \newcommand{\Pa}{\protect\kemtkn{Pa}}
127 \newcommand{\U}{\protect\kemtkn{U}}
128 \newcommand{\Np}{\protect\kemtkn{Np}}
129 \newcommand{\Pu}{\protect\kemtkn{Pu}}
130 \newcommand{\Am}{\protect\kemtkn{Am}}
131 \newcommand{\Cm}{\protect\kemtkn{Cm}}
132 \newcommand{\Bk}{\protect\kemtkn{Bk}}
133 \newcommand{\Cf}{\protect\kemtkn{Cf}}
134 \newcommand{\Es}{\protect\kemtkn{Es}}
135 \newcommand{\Fm}{\protect\kemtkn{Fm}}
136 \newcommand{\Md}{\protect\kemtkn{Md}}
137 \newcommand{\No}{\protect\kemtkn{No}}
138 \newcommand{\Lr}{\protect\kemtkn{Lr}}
139 \newcommand{\Rf}{\protect\kemtkn{Rf}}
140 \newcommand{\Db}{\protect\kemtkn{Db}}
141 \newcommand{\Sg}{\protect\kemtkn{Sg}}
142 \newcommand{\Bh}{\protect\kemtkn{Bh}}
143 \newcommand{\Hs}{\protect\kemtkn{Hs}}
144 \newcommand{\Mt}{\protect\kemtkn{Mt}}

```

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

```
145 \newcommand{\Me}{\protect\kern{Me}}
146 \newcommand{\Et}{\protect\kern{Et}}
147 \newcommand{\Bu}{\protect\kern{Bu}}
148 \newcommand{\OH}{\protect\kern{OH}}
149 \newcommand{\COOH}{\protect\kern{COOH}}
150 \newcommand{\CH}{\protect\kern{CH}}
```

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