# The mhchem Bundle 

Documentation for the $\mathrm{IAT}_{\mathrm{E}} \mathrm{X}$ Packages<br>mhchem v4.09,<br>hpstatement v2.0.0 and<br>rsphrase v3.11<br>Martin Hensel<br>mhchem@MartinHensel.de

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The mhchem package provides commands for typesetting chemical molecular formulae and equations.

The hpstatement package provides commands for the official hazard statements and precautionary statements ( H and P statements) that are used to label chemicals. 1272/2008, GHS.

The rsphrase package provides commands for the official Risk and Safety ( R and S) Phrases that are used to label chemicals.

## Contents

The mhchem Package ..... 4
Preamble ..... 4
Chemical Equations ..... 4
Chemical Formulae ..... 4
Charges ..... 5
Oxidation States ..... 5
Stoichiometric Numbers ..... 5
Nuclides, Isotopes ..... 6
Parenthesis, Brackets, Braces ..... 6
States of Aggregation ..... 7
Unpaired Electrons, Radical Dots ..... 7
Variables like x, n, 2n+1 ..... 7
Greek Characters ..... 8
(Italic) Math ..... 8
Italic Text ..... 9
Escape Parsing, Upright Text ..... 9
Addition Compounds ..... 9
Bonds ..... 9
Reaction Arrows ..... 10
Equation Operators ..... 11
Precipitate and Gas ..... 11
Further Examples ..... 12
Equation Environments ..... 12
Aligning Equations ..... 12
Own Equation Command ..... 13
Splitting the \ce command ..... 14
Comma Example ..... 14
Layer Stacks ..... 15
The Details ..... 15
Fine Tuning ..... 16
Text Font and Math Font ..... 16
Greek Font ..... 17
Arrows ..... 17
Stacked Superscripts and Subscripts ..... 18
Rudimentary TEX4ht (htlatex) support ..... 18
Major Changes. ..... 19
Migrating from version 1 ..... 19
Migrating from version 2 ..... 19
Migrating from version 3 ..... 19
Most Recent Changes ..... 19
The hpstatement Package and the rsphrase Package ..... 21
Usage ..... 21
Most Recent Changes ..... 23
Appendix ..... 24
List of Implemented H and P Statements. ..... 24
List of Implemented R and S Phrases ..... 29

## The mhchem Package

## Preamble

To use mhchem, request it in your document's preamble with the command

## \usepackage[version=4]\{mhchem\}undefined

What about the version=4? During development, I became aware that additional functionality could not be added without changing the user-interface slightly. But what about backward compatibility? I could, of course freeze mhchem and publish an mhchem 2 package. However, I decided to use a parameter in order to switch to the new interface. One can use version=4 for the most-recent version of mhchem, but version=2 to version=1 are still there for existing documents that use an old user-interface of mhchem. Those old documents should still produce the same results. However, spacing might differ slightly.
mhchem needs a couple of other packages. For instance, expl3, amsmath and calc.

## Chemical Equations

$$
\begin{aligned}
& \mathrm{CO}_{2}+\mathrm{C} \longrightarrow 2 \mathrm{CO} \quad \backslash \operatorname{ce}\{\mathrm{CO} 2+\mathrm{C}->2 \mathrm{CO}\} \\
& \mathrm{Hg}^{2+} \xrightarrow{\mathrm{I}^{-}} \mathrm{HgI}_{2} \xrightarrow{\mathrm{I}^{-}}\left[\mathrm{Hg}^{\mathrm{II}} \mathrm{H}^{2-} \quad\right. \text { पce\{Hg^2+ ->[I-] HgI2 } \\
& \left.->[I-]\left[\mathrm{Hg}^{\wedge}\{I I\} I 4\right]^{\wedge} 2-\right\}
\end{aligned}
$$

## Chemical Formulae

| $\mathrm{H}_{2} \mathrm{O}$ | \ce $\{\mathrm{H} 2 \mathrm{O}\}$ |
| :--- | :--- |
| $\mathrm{Sb}_{2} \mathrm{O}_{3}$ | $\backslash \mathrm{ce}\{\mathrm{Sb} 203\}$ |

This works in text mode (even in headings) and in math mode. (For PDF bookmarks you might have to specify a text-only version.)

This is text with $\mathrm{H}_{2} \mathrm{O}$ and $\mathrm{H}_{2} \mathrm{O}$.

```
\sffamily\itshape
This is text with \ce{H2O} and $\ce{H2O}$.
```

For how to fine-tune the font usage, see Fine Tuning

## Charges

$\mathrm{H}^{+} \quad \backslash$ ce $\{\mathrm{H}+\}$
$\mathrm{CrO}_{4}{ }^{2-} \quad \backslash \mathrm{ce}\left\{\mathrm{CrO}^{\wedge}{ }^{\wedge} 2-\right\}$
$\left[\mathrm{AgCl}_{2}\right]^{-} \quad \backslash \mathrm{ce}\{[\mathrm{AgCl2}]-\}$
$Y^{99+} \quad \backslash \operatorname{ce}\left\{Y^{\wedge} 99+\right\}$
$Y^{99+} \quad \backslash \operatorname{ce}\left\{Y^{\wedge}\{99+\}\right\}$
This will work in text mode and math mode. For text, the en-dash will be used as a minus sign.

## Oxidation States

$$
\mathrm{Fe}^{\mathrm{II}} \mathrm{Fe}^{\mathrm{III}}{ }_{2} \mathrm{O}_{4} \quad \backslash \operatorname{ce}\left\{\mathrm{Fe}^{\wedge}\{\mathrm{II}\} \mathrm{Fe}^{\wedge}\{\mathrm{III}\} 204\right\}
$$

## Stoichiometric Numbers

| $2 \mathrm{H}_{2} \mathrm{O}$ | \ce $\{2 \mathrm{H} 2 \mathrm{O}\}$ |
| :--- | :--- |
| $2 \mathrm{H}_{2} \mathrm{O}$ | \ce $\{2 \mathrm{H} 2 \mathrm{O}\}$ |
| $0.5 \mathrm{H}_{2} \mathrm{O}$ | \ce $\{0.5 \mathrm{H} 2 \mathrm{O}\}$ |
| $\frac{1}{2} \mathrm{H}_{2} \mathrm{O}$ | \ce\{1/2H2O\} |
| $(1 / 2) \mathrm{H}_{2} \mathrm{O}$ | \ce $\{(1 / 2) \mathrm{H} 20\} \%$ IUPAC Green Book |
| $n \mathrm{H}_{2} \mathrm{O}$ | \ce\{\$n\$H2O\} |

This works in text mode and math mode. (The fraction line always comes from math mode and might appear too small when using bold text fonts.)

## Nuclides, Isotopes

| ${ }_{90}^{227} \mathrm{Th}^{+}$ | $\backslash \operatorname{ce}\left\{\wedge\{227\} \_\{90\} \mathrm{Th}+\right\}$ |
| :--- | :--- |
| ${ }_{90}^{227} \mathrm{Th}^{+}$ | $\backslash \operatorname{ce}\left\{\wedge 227 \_90 \mathrm{Th}+\right\}$ |
| ${ }_{-1}^{0} \mathrm{n}^{-}$ | $\backslash \operatorname{ce}\left\{\wedge\{0\} \_\{-1\} \mathrm{n}^{\wedge}\{-\}\right\}$ |
| ${ }_{-1}^{0} \mathrm{n}^{-}$ | $\backslash \operatorname{ce}\left\{\wedge 0_{-}-1 \mathrm{n}-\right\}$ |

It might be ambiguous whether a superscript belongs to the left or right letter. You can make sure by hand (using $\}$ ) or leave it to the automatic detection (digits only $=$ mass number $=$ belongs to right side).

| $\mathrm{H}^{3} \mathrm{HO}$ | $\backslash c e\left\{\mathrm{H}\left\}^{\wedge} 3 \mathrm{HO}\right\} \backslash \backslash\right.$ |
| :--- | :--- |
| $\mathrm{H}^{3} \mathrm{HO}$ | $\backslash c e\left\{\mathrm{H}^{\wedge} 3 \mathrm{HO}\right\}$ |

Of course, all of this works in text mode and math mode.

## Parenthesis, Brackets, Braces

Use parenthesis ( ) and brackets [ ] normally. Write braces as <br>{ <br>}.
$\left(\mathrm{NH}_{4}\right)_{2} \mathrm{~S} \quad$ Ice\{(NH4)2S\}
$\left[\left\{\left(\mathrm{X}_{2}\right)_{3}\right\}_{2}\right]^{3+} \quad \backslash \operatorname{ce}\left\{[\backslash\{(\mathrm{X} 2) 3 \backslash\} 2]^{\wedge} 3+\right\}$
Small parenthesis etc. work in both, text mode and math mode. Large parenthesis etc. are a math-mode only feature.

Both, \left and \right macros, need to be in the same math environment, so you might have to put \ce into \$ into \ce, but that's fine.
$\mathrm{CH}_{4}+2\left(\mathrm{O}_{2}+\frac{79}{21} \mathrm{~N}_{2}\right)$
\ce\{CH4 + 2 \$\left ( \ce\{02 + 79/21 N2\} \right) \$\}

## States of Aggregation

| $\mathrm{H}_{2}(\mathrm{aq})$ | $\backslash \mathrm{ce}\{\mathrm{H} 2(\mathrm{aq})\} \%$ IUPAC recommendation |
| :--- | :--- |
| $\mathrm{CO}_{3}{ }^{2-}(\mathrm{aq})$ | $\backslash \mathrm{ce}\left\{\mathrm{CO}^{\wedge} 2-\{ \} \_\{(\mathrm{aq})\}\right\} \%$ not IUPAC-conform |
| $\mathrm{NaOH}(\mathrm{aq}, \infty)$ | $\backslash \mathrm{ce}\{\mathrm{NaOH}(\mathrm{aq}, \$ \backslash$ infty $\$)\}$ |

This works in text mode and math mode.

## Unpaired Electrons, Radical Dots

| $\mathrm{OCO}^{\bullet-}$ | $\backslash \operatorname{ce\{ 0C0^{\wedge }\{ .-\} \} }$ |
| :--- | :--- |
| $\mathrm{NO}^{(2 \bullet)-}$ | $\backslash \operatorname{ce}\left\{\mathrm{NO}^{\wedge}\{(2)-\}.\right\}$ |

This superscript-only feature works in text mode and math mode. A math bullet is used.

## Variables like $\mathbf{x}, \mathbf{n}, \mathbf{2 n + 1}$

Typographical conventions say that variables are typeset in italic font, while other entities (like chemical elements) are typeset in an upright font.
mhchem tries to recognize common patterns and use the correct (italic) font, like the $x$ and $2 n$ in the following examples.

```
NO
Fe}\mp@subsup{}{}{n+}\mp@subsup{F}{e}{n+
x Na(NH4})\mp@subsup{\textrm{HPO}}{4}{}\xrightarrow{}{\Delta}(\mp@subsup{\textrm{NaPO}}{3}{}\mp@subsup{)}{x}{}+x\mp@subsup{\textrm{NH}}{3}{}\uparrow+x\mp@subsup{\textrm{H}}{2}{}\textrm{O
    $\ce{x Na(NH4)HPO4 -> [\Delta] (NaPO3)_x + x NH3 ^ + x H2O}$
```

If a more complex term is not properly recognized, you can switch to math mode (= italics) explicitly.

## Greek Characters

Just write \alpha etc. This works in text mode and math mode.
Typographical conventions say that variables are typeset in italic font, while other entities (like chemical elements) are typeset in an upright font. Here, the Greek character is not a variable that stands for a number, therefore an upright font is used.

```
\mu-Cl \ce{\mu-Cl}
[Pt(\eta}\mp@subsup{\eta}{}{2}-\mp@subsup{\textrm{C}}{2}{}\mp@subsup{\textrm{H}}{4}{})\mp@subsup{\textrm{Cl}}{3}{}\mp@subsup{]}{}{-}\\ce{[Pt(\eta^2-C2H4)Cl3]-
```

If the greek character is followed by a space, you need to type $\}$, otherwise the space will be lost.
${ }_{90}^{234} \mathrm{Th} \longrightarrow{ }_{-1}^{0} \beta+{ }_{91}^{234} \mathrm{~Pa} \backslash \mathrm{ce}\left\{\wedge 234 \_90 \mathrm{Th}->{ }^{\wedge} 0_{-}-1 \backslash\right.$ beta $\left.\{ \}+{ }^{\wedge} 234 \_91 \mathrm{~Pa}\right\}$
By defaut, $\mathrm{AT}_{\mathrm{E}} \mathrm{X}$ does not come with upright Greek characters. Therefore, it is recommended to load a package for that, that visually fits to your font. For more details, see the section Greek Font,

If you need an italic Greek character (i.e. a variable that stands for a number), use math mode like \$\alpha\$.

## (Italic) Math

By using \$. . . \$, you can esacpe to 'font-corrected math mode'.

```
\(\mathrm{NaOH}(\mathrm{aq}, \infty)\)
\(\mathrm{NaOH}(\mathrm{aq}, \infty)\)
\(\mathrm{Fe}(\mathrm{CN}) \frac{6}{2}\)
\(\mathrm{Fe}(\mathrm{CN}) \frac{6}{2}\)
```

```
$\ce{NaOH(aq,$\infty$)}$\\
```

$\ce{NaOH(aq,$\infty$)}$<br>
\sffamily\bfseries
\sffamily\bfseries
\ce{NaOH(aq,$\infty$)}
\ce{NaOH(aq,$\infty$)}
$\ce{Fe(CN)_{$\frac{6}{2}$}}$<br>
$\ce{Fe(CN)_{$\frac{6}{2}$}}$<br>
\sffamily\bfseries
\sffamily\bfseries
\ce{Fe(CN)_{$\frac{6}{2}$}}

```
\ce{Fe(CN)_{$\frac{6}{2}$}}
```

In font-corrected math mode, mhchem regonizes some common patterns and prints them font-corrected (e.g. for use in headings). Otherwise, it will fall back to 'full math mode'.

You can force 'full math mode' with $\$\{. .\} \$.$$ .$
$\mathrm{NO}_{x} \mathbf{N O}_{x}$
\$\ce\{NO_\$\{x\}\$\}\$ \sffamily\bfseries \ce\{NO_\$\{x\}\$\}

## Italic Text

With the same mechanism, you can switch to italic font.


```
\sffamily\bfseries
\ce{$cis${-}[PtCl2(NH3)2]}
```

Spaces will be ignored. Use a $\sim$ when you need to typeset a space.
This works for the text mode as long as you use latin characters. It also works for the math font.

## Escape Parsing, Upright Text

If you want to escape parsing, for instance for a simple hyphen (that should not become a bond), use \{...\}.
$(+)_{589}-\left[\mathrm{Co}(\mathrm{en})_{3}\right] \mathrm{Cl}_{3}$
$(+)_{589}-\left[\mathrm{Co}(\mathrm{en})_{3}\right] \mathrm{Cl}_{3}$

```
\ce{{(+)}_589{-}[Co(en)3]Cl3}\\
\sffamily\bfseries
\ce{{(+)}_589{-}[Co(en)3]Cl3}
```


## Addition Compounds

| $\mathrm{KCr}\left(\mathrm{SO}_{4}\right)_{2} \cdot 12 \mathrm{H}_{2} \mathrm{O}$ | $\backslash \operatorname{ce}\{\mathrm{KCr}(\mathrm{SO} 4) 2 \star 12 \mathrm{H} 20\}$ |
| :--- | :--- |
| $\mathrm{KCr}\left(\mathrm{SO}_{4}\right)_{2} \cdot 12 \mathrm{H}_{2} \mathrm{O}$ | $\backslash \operatorname{ce}\{\mathrm{KCr}(\mathrm{SO} 4) 2.12 \mathrm{H} 20\}$ |
| $\mathrm{KCr}\left(\mathrm{SO}_{4}\right)_{2} \cdot 12 \mathrm{H}_{2} \mathrm{O}$ | $\backslash \operatorname{ce}\{\mathrm{KCr}(\mathrm{SO} 4) 2 \star 12 \mathrm{H} 2 \mathrm{O}\}$ |

The centered dot is taken from math font.

## Bonds

| $\mathrm{C}_{6} \mathrm{H}_{5}-\mathrm{CHO}$ | \ce\{C6H5-CHO\} |
| :--- | :--- |
| $\mathrm{A}-\mathrm{B}=\mathrm{C} \equiv \mathrm{D}$ | \ce\{A-B=C\#D\} |
| $\mathrm{A}-\mathrm{B}=\mathrm{C} \equiv \mathrm{D}$ | $\backslash$ sffamily $\backslash$ bfseries |
|  | $\backslash c e\{\mathrm{~A}-\mathrm{B}=\mathrm{C} \# \mathrm{D}\}$ |

mhchem tries to differentiate whether $\backslash c e\{-\}$ should be a bond, a charge or a hyphen.

The \# bond might not work if you pass it through other commands. In this case, use $\backslash$ bond \{3\} instead.

```
\(\mathrm{A}-\mathrm{B}=\mathrm{C} \equiv \mathrm{D} \quad \backslash \mathrm{ce}\{\mathrm{A} \backslash\) bond \(\{-\} \mathrm{B} \backslash\) bond \(\{=\} \mathrm{C} \backslash\) bond \(\{\#\} \mathrm{D}\}\)
\(\mathrm{A}-\mathrm{B}=\mathrm{C} \equiv \mathrm{D} \quad \backslash \operatorname{ce}\{\mathrm{A} \backslash\) bond \(\{1\} \mathrm{B} \backslash\) bond \(\{2\} \mathrm{C} \backslash\) bond \(\{3\} \mathrm{D}\}\)
\(A \cdots B=C \quad \backslash c e\{A \backslash\) bond \(\{\sim\} B \backslash\) bond \(\{\sim-\} C\}\)
\(A \cong B \equiv C \equiv D \quad \backslash c e\{A \backslash\) bond \(\{\sim--\} B \backslash\) bond \(\{\sim=\} C \backslash\) bond \(\{-\sim-\} D\}\)
\(\mathrm{A} \cdots \mathrm{B} \cdots \mathrm{C} \quad \backslash \mathrm{ce}\{\mathrm{A} \backslash\) bond \(\{\ldots\} \mathrm{B} \backslash\) bond \(\{\ldots . .\} \mathrm{C}\).
\(A \rightarrow B \leftarrow C \quad \backslash c e\{A \backslash\) bond \(\{->\} B \backslash\) bond \(\{<-\} C\}\)
```

Text mode: Line-based bonds are based on the text-font's en-dash. For all the others, math glyphs are used.

Math mode: Bonds are based on the math-font minus sign. All bonds are vertically aligned on the math axis. For most math fonts, this is slightly lower than half the height of a capital letter.

If you switch to another font, the sidebearing of the minus sign may vary, which would cause the dashed bonds to align badly. In that case, adjust the alignment by using the following command with slightly changed values. Use \mhchemoptions \{minus-text-sidebearing-left=0.10em, minus-text-sidebearing-right=0.16em\} for text font adjustment and \mhchemoptions\{minus-math-sidebearing-left=0.06em, minus-math-sidebearing-right=0.11em\} for math font.

## Reaction Arrows

```
A\longrightarrowB \ce{A >> B}
A\longleftarrowB \ce{A<- B}
A \B \ce{A <-> B}% not to be used according to IUPAC
A }\rightleftarrows\textrm{B}\quad\ce{A<-->B
A\rightleftharpoonsB \ce{A <> B}
A B \ce{A<< B}
A\rightleftharpoonsB \ce{A<<<> B}
```

The arrow arguments use the same syntax as the \ce command.


For how you can change the layout of the arrows, see Fine Tuning

## Equation Operators

$A+B \quad \backslash c e\{A+B\}$
A-B $\quad$ Ces $A-B\} \%$ not to be confused with bonds
$\mathrm{A}=\mathrm{B} \quad \backslash \operatorname{ce}\{\mathrm{A}=\mathrm{B}\} \%$ not to be confused with bonds
$\mathrm{A} \pm \mathrm{B} \quad$ \ce\{A \pm B\}

This works in text mode and math mode. The respective font is used, except for $\backslash \mathrm{pm}$, which always come from math font.

## Precipitate and Gas

```
\(\mathrm{SO}_{4}{ }^{2-}+\mathrm{Ba}^{2+} \longrightarrow \mathrm{BaSO}_{4} \downarrow \quad \backslash \mathrm{ce}\left\{\mathrm{SO}^{\wedge}{ }^{\wedge} 2-+\mathrm{Ba} \wedge 2+->\mathrm{BaSO} 4 \mathrm{v}\right\}\)
\(\mathrm{A} \downarrow \mathrm{B} \downarrow \longrightarrow \mathrm{B} \uparrow \mathrm{B} \uparrow \quad \backslash \mathrm{ce}\{\mathrm{A} \vee \mathrm{B}(\mathrm{v}) \rightarrow \mathrm{B} \wedge \mathrm{B}(\wedge)\}\)
```


## Further Examples

```
    \ce{Zn^2+
        <=>[+ 2OH-][+ 2H+]
        $\underset{\text{amphoteres Hydroxid}}{\ce{Zn(OH)2 v}}$
        <=>[+ 2OH-][+ 2H+]
        $\underset{\text{Hydroxozikat}}{\ce{[Zn(OH)4]^2-}}$
    }
Zn}\mp@subsup{\textrm{Z}}{}{2+}\stackrel{+2\mp@subsup{\textrm{OH}}{}{-}}{+2\mp@subsup{\textrm{H}}{}{+}}\underset{\mathrm{ amphoteres Hydroxid}}{\textrm{Zn}(\textrm{OH}\mp@subsup{)}{2}{}\downarrow}\xlongequal{+2\mp@subsup{\textrm{H}}{}{+}}{+2\mp@subsup{\textrm{OH}}{}{-}
    $K = \frac{[\\ce{Hg^2+}][\ce{Hg}]}{[\ce{Hg2^2+}]}$
K=}=\frac{[\mp@subsup{\textrm{Hg}}{}{2+}][\textrm{Hg}]}{[\mp@subsup{\textrm{Hg}}{2}{2+}]
    $K = \ce{\frac{[Hg^2+][Hg]}{[Hg2^2+]}}$
K= [ [\mp@subsup{\textrm{Hg}}{}{2+}][\textrm{Hg}]}[\mp@subsup{\textrm{Hg}}{2}{2+}
    \ce{Hg^2+ -> [I-]
        $\underset{\mathrm{red}}{\ce{HgI2}}$
        ->[I-]
        $\underset{\mathrm{red}}{\ce{[Hg^{II}I4]^2-}}$
    }
Hg}\mp@subsup{}{2+}{+}\xrightarrow{}{\mp@subsup{\textrm{I}}{}{-}}\underset{\mathrm{ red }}{\mp@subsup{\textrm{HgI}}{2}{}}\xrightarrow{}{\mp@subsup{\textrm{I}}{}{-}}\underset{\mathrm{ red }}{[\mp@subsup{\textrm{Hg}}{\mathrm{ II I}}{4}}\mp@subsup{]}{}{2-
```


## Equation Environments

## Aligning Equations

You can use \& and $\backslash \backslash$ inside $\backslash c e$ to align equations.

$$
\begin{aligned}
\mathrm{RNO}_{2} & \stackrel{+\mathrm{e}}{\rightleftharpoons} \mathrm{RNO}_{2}^{-\bullet}
\end{aligned} \begin{array}{r}
\text { \begin\{align } \star \} } \\
{\text { \ce\{RNO2 \&<=>[+e] RNO2^\{-.\} \\
}} \\
{\mathrm{RNO}_{2}{ }^{-\bullet} \stackrel{+\mathrm{e}}{\rightleftharpoons} \mathrm{RNO}_{2}^{2-}}
\end{array} \begin{array}{c}
\text { RNO2^\{-.\} \&<=>[+e] RNO2^2-\}}
\end{array}
\end{array}
$$

## Own Equation Command

When you use equation environments containing a \ce very often, you might want to create your own command. You could-preferably in your preamble-define the following two commands

```
\newcommand\reaction[1]{\begin{equation}\ce{#1}\end{equation}}
\newcommand\reactionnonumber[1]%
    {\begin{equation*}\ce{#1}\end{equation*}}
```

and then use them as follows.

$$
\begin{align*}
& \mathrm{CO}_{2}+\mathrm{C}  \tag{0.1}\\
& \mathrm{CO}_{2}+\mathrm{C}
\end{align*}
$$

```
\reaction{CO2 + C}
\reactionnonumber{CO2 + C}
```

The advanced $\mathrm{LAT}_{\mathrm{E}} \mathrm{X}$ user could replace the two definitions by one

```
\makeatletter
    \newcommand\reaction@[1]{\begin{equation}\ce{#1}\end{equation}}
    \newcommand\reaction@nonumber[1]%
        {\begin{equation*}\ce{#1}\end{equation*}}
    \newcommand\reaction{\@ifstar{\reaction@nonumber}{\reaction@}}
\makeatother
```

and then write

$$
\begin{align*}
& \mathrm{CO}_{2}+\mathrm{C}  \tag{0.2}\\
& \mathrm{CO}_{2}+\mathrm{C}
\end{align*}
$$

```
\reaction{CO2 + C}
\reaction*{CO2 + C}
```

for the same result.

So far, so good. All reactions will be labelled exactly as all the equations. A few people asked for a different set of numbers for equations and reactions. One could use this code:

```
\makeatletter
\newcounter{reaction}
%%% >> for article <<
%\renewcommand\thereaction{C\,\arabic{reaction}}
%%% << for article <<
```

```
%%% >> for report and book >>
\renewcommand\thereaction{C\,\thechapter.\arabic{reaction}}
\@addtoreset{reaction}{chapter}
%%% << for report and book <<
\newcommand\reactiontag%
    {\refstepcounter{reaction}\tag{\thereaction}}
\newcommand\reaction@[2][]%
    {\begin{equation}\ce{#2}%
    \ifx\@empty#1\@empty\else\label{#1}\fi%
    \reactiontag\end{equation}}
\newcommand\reaction@nonumber[1]%
    {\begin{equation*}\ce{#1}\end{equation*}}
\newcommand\reaction%
    {\@ifstar{\reaction@nonumber}{\reaction@}}
\makeatother
```

With that, all reactions will be labelled independently of the equations.

$$
\begin{equation*}
a+b \tag{0.3}
\end{equation*}
$$

$$
\begin{align*}
& \mathrm{CO}_{2}+\mathrm{C}  \tag{CC1.1}\\
& \mathrm{CO}_{2}+\mathrm{C} \\
& \mathrm{CO}_{2}+\mathrm{C}
\end{align*}
$$

\begin\{equation\}a+b\end\{equation\} }
\reaction\{CO2 + C\}
$\backslash$ reaction*\{CO2 + C\}
\reaction[react:co] \{CO2 + C\}
$\backslash$ begin\{equation\}a+b\end\{equation\} }
$a+b$

## Splitting the \ce command

As mentioned before, you can use \$ to switch to math mode inside \ce. But maybe, you want to 'escape' to outside of \ce.

## Comma Example

Assume, you are getting tired of typing

```
\(\mathrm{N}_{2}, \mathrm{O}_{2}, \mathrm{CO}_{2} \backslash \mathrm{ce}\{\mathrm{N} 2\}, \backslash \mathrm{ce}\{02\}, \backslash \mathrm{ce}\{\mathrm{CO} 2\}\)
```

Then you could define your own command that splits at commas (plus space).

```
\(\mathrm{N}_{2}, \mathrm{O}_{2}, \mathrm{CO}_{2}\)
\newcommand*\cec[1]\{\cesplit\{\{\, \ \(\}\{\backslash 0\}\}\{\# 1\}\}\)
\cec\{N2, 02, CO2\}
```

You could re-define \ce with \newcommand*\ce\{\cesplit\{...\}\{\#1\}\}, if you do not like to create a new name.

## Layer Stacks

Another example shows how physicists can use mhchem to write layer stacks.

```
\newcommand*\stackslash{\text{/}\allowbreak}
\newcommand*\stackhyphen{\text{-}\allowbreak}
\newcommand\stack[1]{%
    \cesplit{%
        {\/}{\c{stackslash}}%
        {-}{\c{stackhyphen}}%
    } {#1}%
}
\ldots\ structure of
\stack{Co-Fe-B/HfO2/Co-Fe-B} is resp\ldots
```


## The Details

\cesplit takes two parameters. The first one is a list of search-and-replace pairs, the second parameter is the chemistry string as you would put into \ce. The search-andreplace list uses the syntax of $l 3$ regex. As a rule of thumb, precede every non-letter with a backslash. You can replace it with some other text, or use $\backslash 0$ to retain the match. If you want to replace with a macro, write $\backslash c\{$ macroname $\}$. For further details, refer to the 13 regex manual.

Do not nest \cesplit commands.
The result of $\backslash$ cesplit does not have the feature to use \& and $\backslash \backslash$ as you might to want to deal with them differently. \ce is itself defined by \cesplit (which, technically speaking, does not split \ce, but an internal command). As \ce is defined by

```
\cesplit % spaced added for readability
    {
        { \c{\\}(\\.*?\])? } { \0 }
        { \& } { \0 }
    }
    {#1}
```

you could add these rules to you own \cesplit definition.

## Fine Tuning

All options explained here, can either be set using the ionscommand\mhchemoptions\{arrows=pgf\}orasoptionstothepackage\usepackage[version=4,arrows=pgf]\{mhchem\}undefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefined

## Text Font and Math Font

mhchem uses the current text font (if you use \ce in text mode) or the current math font (if you use \ce in math mode). If you want, however, you can set a font that will be used for all your formulae and equations.

Inside your document, you can use

```
\mhchemoptions{textfontcommand=\sffamily}
\mhchemoptions{mathfontcommand=\mathsf}
```

in order to get sanf-serif fonts in both, text mode and math mode.
You can use any font command there, not only the mentioned ones. Please be aware that the text-font command is a font switching command (taking no arguments) while the math-font command takes one argument and typesets it.

You can specify the commands by name only, i.e. without the $\backslash$.

```
\mhchemoptions{textfontname=sffamily}
\mhchemoptions{mathfontname=mathsf}
```

Only the latter options can be used with the gecommand,becausethefontcommandsarenotproperlydefinedinthepreamble,yet.Theshortcut$\backslash$mhchemoptions$\{\mathbf{font}=\mathbf{sf}\}$setsthetwofontstosans-serif,asmentionedabove,and\mhchemoptions\{font=\}switchesbacktothedefault,whichisequivalentto\mhchemoptions\{textfontcommand=,mathfontcommand=\mathrm\}undefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefined

## Greek Font

If you load a package for upright Greek characters, this will automatically be used. You can load any of the following packages (e.g. }inthepreamble).Choosetheonethatvisuallyfitsyourfont.undefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefined

- textgreek,
- upgreek,
- newtx,
- kpfonts,
- mathdesign,
- fourier,
- textalpha,
- fontspec.

This functionality was possible by the very neat chemgreek package of Clemens Niederberger. If you want to have different Greek fonts for text mode and math mode, you can specify these 'mappings' by (for instance) \mhchemoptions\{textgreek=upgreek, math-greek=default\}. You can use any of the package names from above, or default or var-default. Refer to the chemgreek manual for details (in particular its Appendix 'Overviews Over the Mappings').

## Arrows

By default, mhchem uses arrows that are composed of different math-font characters, because it uses some features of the amsmath package.

```
\(A \rightleftarrows B\)
\mhchemoptions\{arrows=font\}\% default
\ce\{A <--> B\}
```

But you may switch to arrows drawn with PGF (using TikZ). These are activated by

```
\usepackage[version=3,arrows=pgf]{mhchem}
% or
\usepackage[version=3,arrows=pgf-filled]{mhchem}
```

The tikz package is loaded automatically if you switch to PGF arrows in the preamble (as you do when using itchinsideyourdocument(with\mhchemoptions),don'tforgettoloadtherequiredpackagesmanuallyinyourpreamble:\RequirePackage\{tikz\}\usetikzlibrary\{arrows.meta\}.$A\rightleftarrowsB$undefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefined

```
\mhchemoptions{arrows=pgf}
\ce{A <--> B}
\mhchemoptions{arrows=pgf-filled}
\ce{A <--> B}
```

You can select other pre-defined PGF arrows (see PGF manual) or even define your own. Activate them with the option pgf=\{arrow-name\}\{line-width\}. The dimensions of your custom arrows are expected to be close to those of the built-in mhchem arrows. By the way, they have line width of 0.09 ex .

```
\mhchemoptions{arrows=%
A }\rightleftarrows\textrm{B}\quad\operatorname{pgf{Kite[length=0pt 4,width'=0pt 1]}{0.15ex}}
\ce{A <--> B}
```


## Stacked Superscripts and Subscripts

```
CrO
    \mhchemoptions{layout=staggered-flat}% default
    \ce{CrO4^2-}
    \mhchemoptions{layout=staggered-deep}
CrO
    \ce{CrO4^2-}
    \mhchemoptions{layout=stacked}
    \ce{CrO4^2-} % not IUPAC-conform
```


## Rudimentary TEX4ht (htlatex) support

mhchem has basic support for $\mathrm{T}_{\mathrm{E}} \mathrm{X} 4$ ht (htlatex). Summary formulae should work fine. Special bonds and reaction arrows are recognizable, but ugly. Complex math with mhchem inside might fail completely.

## Major Changes

## Migrating from version 1

Inner - characters are considered to be bonds. Use \$. . . $\$$ for math mode inside $\backslash c e$ (no braces any more).

## Migrating from version 2

Meaning and usage of \bond changed.

## Migrating from version 3

The arrow arguments are set with the same syntax as the \ce command-use $\$ \ldots$. . or $\$\{\ldots\} \$$ for math. Deprecated commands like \cf, , and ' and \hyphen and \cmath were removed completely. \cee was removed-just use \ce. \{....\} does escape to text now, not math. \$. . . \$ does only escape to 'font-corrected math mode'—check the results. Additional spaces will be inserted: A $\$ x \backslash$, $\mathbf{H} 20$ should be changed to $\$ x \$ \mathrm{H} 20$. Appearance of bonds, radical dot, $x$, single-letter variables, - in subscripts etc. slightly changed-check if this fits with your font, in particular your text font. Check all complex subscripts and superscripts (more than just number or a charge).

## Most Recent Changes

2021-12-31 mhchem v4.09

- Bring back lost TeX4ht support

2018-06-22 mhchem v4.08

- Work around unicode-math incompatibilities

2017-07-24 mhchem v4.07

- Adapt to $\mathrm{LAT}_{\mathrm{E}} \mathrm{X} 3(\operatorname{expl} 3)$ changes


## 2017-01-16 mhchem v4.06

- Adapt to upcoming $\mathrm{EAT}_{\mathrm{E}} \mathrm{X} 3$ change


## 2016-08-07 mhchem v4.05

- extended variable recognition - single lower-case letters in superscripts/subscripts are typeset in an italic font
- improved bond/charge/hyphen distinction
- fixed error handling for nonstopmode


## 2016-02-07 mhchem v4.04

- support for negative subscripts, \ce\{^0_-1n-\}
- \frac\{\} \{\} added
- \$ \alpha\$ fixed (math Greek)


## 2015-11-29 mhchem v4.03

- reworked arrows and provided option for custom pgf arrows
- improved speed

2015-07-23 mhchem v4.02

- added rudimentary TeX4ht support
- fixed the \str_case:nnn bug-expl3 removed that function


## 2015-04-23 mhchem v4.01

- support upright greek characters (chemgreek)
- syntax improvements
- recognition of states of aggregation
- text-font operators + , -, =


## 2015-04-07 mhchem v4.00

- many syntax improvements
- many layout improvements
- stricter distinction between text font and math font, many math features are translated into their text equivalent, e.g. italic variables
- new options
- removed deprecated commands


## The hpstatement Package and the rsphrase Package

The hpstatement package contains all official hazard statements and precautionary statements (H and P) of the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) and of the CLP Regulation of the European Union.

The statements are fully supported in English, French, and German. For other languages, just the base forms are available.

The rsphrase package contains the text of all official Risk and Safety (R and S) Phrases that were used to label chemicals.

These phrases are available in Danish, Englisch, French, German, Spanish, and Italian.

Please be advised that, as stated in the license, the authors provide no warranty of correctness.

## Usage

The hpstatement package contains all text versions published by the European Parliament. Load the package with tatement\}togetthemost-recentversions.Orloadwith\usepackage[date=2021-01-01]\{hpstatement\}togettextsofacertaindateandkeepthedocumentstableevenafteranupdate.Incaseyouwouldneedtoswitchwithinadocument,use\hpsetup\{date=2021-01-01\}.undefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefinedundefined

The package provides two commands: \hpstatement and \hpnumber. \hpstatement inserts the statement's text, \hpnumber its formatted number.

The statement H200
is 'Unstable explosives.'

The statement $\backslash$ hpnumber $\{\mathrm{H} 200\} \backslash \backslash$
is ' $\backslash$ hpstatement $\{\mathrm{H} 200\}$ '

One can use the two commands with an empty argument. It is then assumed that the argument is equivalent to the one used previously.

```
The statement H200
is 'Unstable explosives.'
```

```
The statement \hpnumber{H200}\\
```

The statement \hpnumber{H200}<br>
is '\hpstatement{}'

```
is '\hpstatement{}'
```

The commands add text in your currently selected language.

```
H200: Instabil, explosiv.
```

\selectlanguage\{ngerman\}\% babel
\hpnumber\{H200\}:
\hpstatement\{\}

Some phrases allow you to choose between certain alternatives. In these cases, special numbers (<number>.1, <number>.2, ...) are available for \hpstatement. Of course, the official number is typeset if you call $\backslash$ hpnumber with a special number.

```
P241: Use explosion-proof ventilating \hpnumber{P241.2}:
equipment. \hpstatement{}
```

For phrases with selection, an additional special number is provided that refers to the base form as stated in the regulations: <number>. 0 (e.g. P241.0).

```
P241: Use explosion-proof [electrical/
ventilating/lighting/...] equipment. \hpstatement {}
```

Some statements refer to 'this label'. If you are creating documents that are not labels, you might want to rephrase this. You can do so, by using the (unofficial) <number>.nolabel statement (e.g. P321.nolabel).

See the appendix for a complete list of all implemented English statements, including all options.

The rsphrase package has no date option, but otherwise works the same way, and provides the commands $\backslash$ rsnumber and $\backslash$ rsphrase.

Source of the H and P statements: This project contains data extracted from The Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures ('CLP regulation’), from https://eur-lex.europa.eu. enhanced by individual contributors. This work is licensed under the Creative Commons Attribution 4.0 International licence https://creativecommons.org/licenses/by/4.0/). This means that you can re-use
the content provided you acknowledge the source and indicate any changes you have made. The data is not necessarily comprehensive, complete, accurate or up to date. The acknowledgement is not needed when using statements of the data set for labelling products, of course, as this is the intended usage. © European Union, https: //eur-lex.europa.eu 1998-2021, CC BY 4.0, © hpstatements contributors, https://github.com/mhchem/hpstatements/contributors 2019-2021, CC BY 4.0

Sources for the R and S phrases were documents downloaded from http://europa.eu.int previously to be found under http://europa.eu.int/comm/environment/dansub/pdfs/annex3_en.pdf and http://europa.eu.int/comm/environment/dansub/pdfs/annex4_en.pdffwhich in turn were linked from/http://europa.eu.int/comm/environment/dansub/main67_548/index_en.htm

## Most Recent Changes

## 2021-12-31 hpstatement v2.0.0

- Using most-recent statements from the EU
- Adding date option and all statements in all versions ever published by the EU
- Enhanced statements just for English, French, German


## Appendix

## List of Implemented H and P Statements

These statements are available in English, French, and German.

For other languages, just the base forms are available, e. g. P241, but not P241.0, P241.1, etc. A package update that brings full support might lead to an error message that will be easy to fix. If you are a native speaker of either Bulgarian, Czech, Danish, Dutch, Estonian, Finnish, Greek, Hungarian, Irish, Italian, Latvian, Lithuanian, Maltese, Polish, Portuguese, Romanian, Slovak, Slovenian, Spanish or Swedish, and would like to help offering the statements in those languages, please contact the author. It's not much work to do.

The statements are available in all the versions published by the European Union. Oldest version: 2008-12-16. Newest version: 2021-10-01.

H200 (H200): Unstable explosives. H201 (H201): Explosive; mass explosion hazard. H202 (H202): Explosive, severe projection hazard. H203 (H203): Explosive; fire, blast or projection hazard. H204 (H204): Fire or projection hazard. H205 (H205): May mass explode in fire. H206 (H206): Fire, blast or projection hazard; increased risk of explosion if desensitising agent is reduced. H207 (H207): Fire or projection hazard; increased risk of explosion if desensitising agent is reduced. H208 (H208): Fire hazard; increased risk of explosion if desensitising agent is reduced. H220 (H220): Extremely flammable gas. H221 (H221): Flammable gas. H222 (H222): Extremely flammable aerosol. H223 (H223): Flammable aerosol. H224 (H224): Extremely flammable liquid and vapour. H225 (H225): Highly flammable liquid and vapour. H226 (H226): Flammable liquid and vapour. H228 (H228): Flammable solid. H229 (H229): Pressurised container: May burst if heated. H230 (H230): May react explosively even in the absence of air. H231 (H231): May react explosively even in the absence of air at elevated pressure and/or temperature. H232 (H232): May ignite spontaneously if exposed to air. H240 (H240): Heating may cause an explosion. H241 (H241): Heating may cause a fire or explosion. H242 (H242): Heating may cause a fire. H250 (H250): Catches fire spontaneously if exposed to air. H251 (H251): Self-heating: may catch fire. H252 (H252): Selfheating in large quantities; may catch fire. H260 (H260): In contact with water releases flammable gases which may ignite spontaneously. H261 (H261): In contact with water releases flammable gases. H270 (H270): May cause or intensify fire; oxidiser. H271 (H271): May cause fire or explosion; strong oxidiser. H272 (H272): May intensify fire; oxidiser. H280 (H280): Contains gas under pressure; may explode if heated. H281 (H281): Contains refrigerated gas; may cause cryogenic burns or injury. H290 (H290): May be corrosive to metals. H300 (H300): Fatal if swallowed. H301 (H301): Toxic if swallowed. H302 (H302): Harmful if swallowed. H304 (H304): May be fatal if swallowed and enters airways. H310 (H310): Fatal in contact with skin. H311 (H311): Toxic in contact with skin. H312 (H312): Harmful in contact with
skin. H314 (H314): Causes severe skin burns and eye damage. H315 (H315): Causes skin irritation. H317 (H317): May cause an allergic skin reaction. H318 (H318): Causes serious eye damage. H319 (H319): Causes serious eye irritation. H330 (H330): Fatal if inhaled. H331 (H331): Toxic if inhaled. H332 (H332): Harmful if inhaled. H334 (H334): May cause allergy or asthma symptoms or breathing difficulties if inhaled. H335 (H335): May cause respiratory irritation. H336 (H336): May cause drowsiness or dizziness. H340.0 (H340): May cause genetic defects <state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>. H340[] (H340): May cause genetic defects. H340[abc] (H340): May cause genetic defects[abc]. H341.0 (H341): Suspected of causing genetic defects <state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>. H341[] (H341): Suspected of causing genetic defects. H341[abc] (H341): Suspected of causing genetic defects[abc]. H350.0 (H350): May cause cancer <state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>. H350[] (H350): May cause cancer. H350[abc] (H350): May cause cancer[abc]. H350i (H350i): May cause cancer by inhalation. H351.0 (H351): Suspected of causing cancer <state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>. H351[] (H351): Suspected of causing cancer. H351[abc] (H351): Suspected of causing cancer[abc]. H360.0 (H360): May damage fertility or the unborn child <state specific effect if known > <state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>. H360[] (H360): May damage fertility or the unborn child. H360[abc] (H360): May damage fertility or the unborn child[abc]. H360F (H360F): May damage fertility. H360D (H360D): May damage the unborn child. H360FD (H360FD): May damage fertility. May damage the unborn child. H360Fd (H360Fd): May damage fertility. Suspected of damaging the unborn child. H360Df (H360Df): May damage the unborn child. Suspected of damaging fertility. H361.0 (H361): Suspected of damaging fertility or the unborn child <state specific effect if known> <state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>. H361[] (H361): Suspected of damaging fertility or the unborn child. H361[abc] (H361): Suspected of damaging fertility or the unborn child[abc]. H361f (H361f): Suspected of damaging fertility. H361d (H361d): Suspected of damaging the unborn child. H361fd (H361fd): Suspected of damaging fertility. Suspected of damaging the unborn child. H362 (H362): May cause harm to breast-fed children. H370.0 (H370): Causes damage to organs <or state all organs affected, if known> <state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>. H370.1 (H370): Causes damage to organs. H370.1[def] (H370): Causes damage to organs[def]. H370[abc] (H370): Causes damage to [abc]. H370[abc][def] (H370): Causes damage to [abc][def]. H371.0 (H371): May cause damage to organs <or state all organs affected, if known> <state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>. H371.1 (H371): May cause damage to organs. H371.1[def] (H371): May cause damage to organs[def]. H371[abc] (H371): May cause damage to [abc]. H371[abc][def] (H371): May cause damage to [abc][def]. H372.0 (H372): Causes damage to organs <or state all organs affected, if known> through prolonged or repeated exposure <state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>. H372.1 (H372): Causes damage to organs through prolonged or repeated exposure. H372.1[def] (H372): Causes damage to organs[def]. H372[abc] (H372): Causes damage to [abc] through prolonged or repeated exposure. H372[abc][def] (H372): Causes damage to [abc][def]. H373.0 (H373): May cause damage to organs <or state all organs affected, if known> through prolonged or repeated exposure <state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>. H373.1 (H373): May cause damage to organs through prolonged or repeated exposure. H373.1[def] (H373): May cause damage to organs[def]. H373[abc] (H373): May cause damage to [abc] through prolonged or repeated exposure. H373[abc][def] (H373): May cause damage to [abc][def]. $\mathbf{H 3 0 0 + H 3 1 0}$ (H300 + H310): Fatal if swallowed or in contact with skin H300+H310+H330 (H300 + H310 + H330): Fatal if swallowed, in contact with skin or if inhaled H300+H330 (H300 + H330): Fatal if swallowed or if inhaled H301+H311 (H301 + H311): Toxic if swallowed or in contact with skin H301+H311+H331 (H301 + H311 + H331): Toxic if swallowed, in contact with skin or if inhaled H301+H331 (H301 + H331): Toxic if swallowed or if inhaled H302+H312 (H302 + H312): Harmful if swallowed or in contact with
skin H302+H312+H332 (H302 + H312 + H332): Harmful if swallowed, in contact with skin or if inhaled H302+H332 (H302 + H332): Harmful if swallowed or if inhaled H310+H330 (H310 + H330): Fatal in contact with skin or if inhaled $\mathbf{H 3 1 1}+\mathbf{H} 331(H 311+$ H331): Toxic in contact with skin or if inhaled H312+H332 (H312 + H332): Harmful in contact with skin or if inhaled H400 (H400): Very toxic to aquatic life. H410 (H410): Very toxic to aquatic life with long lasting effects. H411 (H411): Toxic to aquatic life with long lasting effects. H412 (H412): Harmful to aquatic life with long lasting effects. H413 (H413): May cause long lasting harmful effects to aquatic life. H420 (H420): Harms public health and the environment by destroying ozone in the upper atmosphere EUH014 (EUH014): Reacts violently with water. EUH018.0 (EUH018): In use may form flammable/explosive vapour-air mixture. EUH018.1 (EUH018): In use may form flammable vapour-air mixture. EUH018.2 (EUH018): In use may form explosive vapour-air mixture. EUH019 (EUH019): May form explosive peroxides. EUH029 (EUH029): Contact with water liberates toxic gas. EUH031 (EUH031): Contact with acids liberates toxic gas. EUH032 (EUH032): Contact with acids liberates very toxic gas. EUH044 (EUH044): Risk of explosion if heated under confinement. EUH066 (EUH066): Repeated exposure may cause skin dryness or cracking. EUH070 (EUH070): Toxic by eye contact. EUH071 (EUH071): Corrosive to the respiratory tract. EUH201 (EUH201): Contains lead. Should not be used on surfaces liable to be chewed or sucked by children. EUH201A (EUH201A): Warning! Contains lead. EUH202 (EUH202): Cyanoacrylate. Danger. Bonds skin and eyes in seconds. Keep out of the reach of children. EUH203 (EUH203): Contains chromium (VI). May produce an allergic reaction. EUH204 (EUH204): Contains isocyanates. May produce an allergic reaction. EUH205 (EUH205): Contains epoxy constituents. May produce an allergic reaction. EUH206 (EUH206): Warning! Do not use together with other products. May release dangerous gases (chlorine). EUH207 (EUH207): Warning! Contains cadmium. Dangerous fumes are formed during use. See information supplied by the manufacturer. Comply with the safety instructions. EUH208.0 (EUH208): Contains <name of sensitising substance>. May produce an allergic reaction. EUH208[abc] (EUH208): Contains [abc]. May produce an allergic reaction. EUH209 (EUH209): Can become highly flammable in use. EUH209A (EUH209A): Can become flammable in use. EUH210 (EUH210): Safety data sheet available on request. EUH211 (EUH211): Warning! Hazardous respirable droplets may be formed when sprayed. Do not breathe spray or mist. EUH212 (EUH212): Warning! Hazardous respirable dust may be formed when used. Do not breathe dust. EUH401 (EUH401): To avoid risks to human health and the environment, comply with the instructions for use. P101 (P101): If medical advice is needed, have product container or label at hand. P102 (P102): Keep out of reach of children. P103 (P103): Read label before use. P201 (P201): Obtain special instructions before use. P202 (P202): Do not handle until all safety precautions have been read and understood. P210 (P210): Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. P211 (P211): Do not spray on an open flame or other ignition source. P212 (P212): Avoid heating under confinement or reduction of the desensitising agent. P220 (P220): Keep away from clothing and other combustible materials. P222 (P222): Do not allow contact with air. P223 (P223): Do not allow contact with water. P230.0 (P230): Keep wetted with... P230[abc] (P230): Keep wetted with [abc] P231.0 (P231): Handle and store contents under inert gas/... P231.1 (P231): Handle and store contents under inert gas P231[abc] (P231): Handle and store contents under [abc] P232 (P232): Protect from moisture. P233 (P233): Keep container tightly closed. P234 (P234): Keep only in original packaging. P235 (P235): Keep cool. P240 (P240): Ground and bond container and receiving equipment. P241.0 (P241): Use explosion-proof [electrical/ventilating/ lighting/...] equipment. P241.1 (P241): Use explosion-proof electrical equipment. P241.2 (P241): Use explosion-proof ventilating equipment. P241.3 (P241): Use explosion-proof lighting equipment. P242 (P242): Use non-sparking tools. P243 (P243): Take action to prevent static discharges. P244 (P244): Keep valves and fittings free from oil and grease. P250.0 (P250): Do not subject to grinding/shock/friction/ ... . P250.1 (P250): Do not subject to grinding. P250.2 (P250): Do not subject to shock. P250.3 (P250): Do not subject to friction. P251 (P251): Do not pierce or burn, even after use. P260.0 (P260): Do not breathe dust/fume/gas/mist/vapours/spray. P260.1 (P260): Do not breathe dust. P260.2 (P260): Do not breathe fume. P260.3 (P260): Do not breathe gas. P260.4 (P260): Do not breathe mist. P260.5 (P260): Do not
breathe vapours. P260.6 (P260): Do not breathe spray. P261.0 (P261): Avoid breathing dust/fume/gas/ mist/vapours/spray. P261.1 (P261): Avoid breathing dust. P261.2 (P261): Avoid breathing fume. P261.3 (P261): Avoid breathing gas. P261.4 (P261): Avoid breathing mist. P261.5 (P261): Avoid breathing vapours. P261.6 (P261): Avoid breathing spray. P262 (P262): Do not get in eyes, on skin, or on clothing. P263 (P263): Avoid contact during pregnancy and while nursing. P264.0 (P264): Wash ... thoroughly after handling. P264[abc] (P264): Wash [abc] thoroughly after handling. P270 (P270): Do not eat, drink or smoke when using this product. P271 (P271): Use only outdoors or in a well-ventilated area. P272 (P272): Contaminated work clothing should not be allowed out of the workplace. P273 (P273): Avoid release to the environment. P280.0 (P280): Wear protective gloves/protective clothing/eye protection/face protection. P280.1 (P280): Wear protective gloves. P280.2 (P280): Wear protective clothing. P280.3 (P280): Wear eye protection. P280.4 (P280): Wear face protection. P282 (P282): Wear cold insulating gloves and either face shield or eye protection. P283 (P283): Wear fire resistant or flame retardant clothing. P284 (P284): [In case of inadequate ventilation] wear respiratory protection. P231+P232.0 (P231 + P232): Handle and store contents under inert gas/.... Protect from moisture. P231+P232.1 (P231 + P232): Handle and store contents under inert gas. Protect from moisture. P231+P232[abc] (P231 + P232): Handle and store contents under [abc]. Protect from moisture. P301 (P301): IF SWALLOWED: P302 (P302): IF ON SKIN: P303 (P303): IF ON SKIN (or hair): P304 (P304): IF INHALED: P305 (P305): IF IN EYES: P306 (P306): IF ON CLOTHING: P308 (P308): IF exposed or concerned: P310.0 (P310): Immediately call a POISON CENTER/ doctor/... P310.1 (P310): Immediately call a POISON CENTER P310.2 (P310): Immediately call a doctor P310[abc] (P310): Immediately call [abc] P311.0 (P311): Call a POISON CENTER/doctor/... P311.1 (P311): Call a POISON CENTER P311.2 (P311): Call a doctor P311[abc] (P311): Call [abc] P312.0 (P312): Call a POISON CENTRE/doctor/... if you feel unwell. P312.1 (P312): Call a POISON CENTRE/ if you feel unwell. P312.2 (P312): Call a doctor if you feel unwell. P312[abc] (P312): Call [abc] if you feel unwell. P313 (P313): Get medical advice/attention. P314 (P314): Get medical advice/attention if you feel unwell. P315 (P315): Get immediate medical advice/attention. P320.0 (P320): Specific treatment is urgent (see ... on this label). P320[abc] (P320): Specific treatment is urgent (see [abc] on this label). P320.nolabel[abc] (non-official) (P320.nolabel): Specific treatment is urgent (see [abc]). P321.0 (P321): Specific treatment (see ... on this label). P321[abc] (P321): Specific treatment (see [abc] on this label). P321.nolabel[abc] (non-official) (P321.nolabel): Specific treatment (see [abc]). P330 (P330): Rinse mouth. P331 (P331): Do NOT induce vomiting. P332 (P332): If skin irritation occurs: P333 (P333): If skin irritation or rash occurs: P334.0 (P334): Immerse in cool water [or wrap in wet bandages]. P334.1 (P334): Immerse in cool water. P334.2 (P334): Immerse in cool water or wrap in wet bandages. P335 (P335): Brush off loose particles from skin. P336 (P336): Thaw frosted parts with lukewarm water. Do no rub affected area. P337 (P337): If eye irritation persists: P338 (P338): Remove contact lenses, if present and easy to do. Continue rinsing. P340 (P340): Remove person to fresh air and keep comfortable for breathing. P342 (P342): If experiencing respiratory symptoms: P351 (P351): Rinse cautiously with water for several minutes. P352.0 (P352): Wash with plenty of water/... P352.1 (P352): Wash with plenty of water P352[abc] (P352): Wash with [abc] P353.0 (P353): Rinse skin with water [or shower]. P353.1 (P353): Rinse skin with water. P353.2 (P353): Rinse skin with water or shower. P360 (P360): Rinse immediately contaminated clothing and skin with plenty of water before removing clothes. P361 (P361): Take off immediately all contaminated clothing. P362 (P362): Take off contaminated clothing. P363 (P363): Wash contaminated clothing before reuse. P364 (P364): And wash it before reuse. P370 (P370): In case of fire: P371 (P371): In case of major fire and large quantities: P372 (P372): Explosion risk. P373 (P373): DO NOT fight fire when fire reaches explosives. P375 (P375): Fight fire remotely due to the risk of explosion. P376 (P376): Stop leak if safe to do so. P377 (P377): Leaking gas fire: Do not extinguish, unless leak can be stopped safely. P378.0 (P378): Use... to extinguish. P378[abc] (P378): Use [abc] to extinguish. P380 (P380): Evacuate area. P381 (P381): In case of leakage, eliminate all ignition sources. P390 (P390): Absorb spillage to prevent material damage. P391 (P391): Collect spillage. P301+P310.0 (P301 + P310): IF SWALLOWED: Immediately call a POISON CENTER/doctor/... P301+P310.1 (P301 + P310): IF SWALLOWED: Immediately call a POISON CENTER

P301+P310.2 (P301 + P310): IF SWALLOWED: Immediately call a doctor P301+P310[abc] (P301 + P310): IF SWALLOWED: Immediately call [abc] P301+P312.0 (P301 + P312): IF SWALLOWED: Call a POISON CENTRE/doctor/... if you feel unwell. P301+P312.1 (P301 + P312): IF SWALLOWED: Call a POISON CENTRE if you feel unwell. P301+P312.2 (P301 + P312): IF SWALLOWED: Call a doctor if you feel unwell. P301+P312[abc] (P301 + P312): IF SWALLOWED: Call [abc] if you feel unwell. P301+P330+P331 (P301 + P330 + P331): IF SWALLOWED: Rinse mouth. Do NOT induce vomiting. P302+P334 (P302 + P334): IF ON SKIN: Immerse in cool water or wrap in wet bandages. P302+P335+P334.0 (P302 + P335 + P334): IF ON SKIN: Brush off loose particles from skin. Immerse in cool water [or wrap in wet bandages]. P302+P335+P334.1 (P302 + P335 + P334): IF ON SKIN: Brush off loose particles from skin. Immerse in cool water. P302+P335+P334.2 (P302 + P335 + P334): IF ON SKIN: Brush off loose particles from skin. Immerse in cool water or wrap in wet bandages. P302+P352.0 (P302 + P352): IF ON SKIN: Wash with plenty of water/... P302+P352.1 (P302 + P352): IF ON SKIN: Wash with plenty of water P302+P352[abc] (P302 + P352): IF ON SKIN: Wash with [abc] P303+P361+P353.0 (P303 + P361 + P353): IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water [or shower]. P303+P361+P353.1 (P303 + P361 + P353): IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water. P303+P361+P353.2 (P303 + P361 + P353): IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower. P304+P340 (P304+P340): IF INHALED: Remove person to fresh air and keep comfortable for breathing. P305+P351+P338 (P305 + P351 + P338): IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. P306+P360 (P306 + P360): IF ON CLOTHING: rinse immediately contaminated clothing and skin with plenty of water before removing clothes. P308+P311.0 (P308 + P311): IF exposed or concerned: Call a POISON CENTER/doctor/... P308+P311.1 (P308 + P311): IF exposed or concerned: Call a POISON CENTER P308+P311.2 (P308 + P311): IF exposed or concerned: Call a doctor P308+P311[abc] (P308 + P311): IF exposed or concerned: Call [abc] P308+P313 (P308 + P313): IF exposed or concerned: Get medical advice/ attention. P332+P313 (P332 + P313): If skin irritation occurs: Get medical advice/attention. P333+P313 (P333 + P313): If skin irritation or rash occurs: Get medical advice/attention. P336+P315 (P336 + P315): Thaw frosted parts with lukewarm water. Do not rub affected area. Get immediate medical advice/attention. P337+P313 (P337 + P313): If eye irritation persists: Get medical advice/attention. P342+P311.0 (P342 + P311): If experiencing respiratory symptoms: Call a POISON CENTER/doctor/... P342+P311.1 (P342 + P311): If experiencing respiratory symptoms: Call a POISON CENTER P342+P311.2 (P342 + P311): If experiencing respiratory symptoms: Call a doctor $\mathbf{P} 342+\mathrm{P} 311[\mathbf{a b c}](\mathrm{P} 342+\mathrm{P} 311)$ : If experiencing respiratory symptoms: Call [abc] P361+P364 (P361 + P364): Take off immediately all contaminated clothing and wash it before reuse. P362+P364 (P362 + P364): Take off contaminated clothing and wash it before reuse. P370+P372+P380+P373 (P370 + P372 + P380 + P373): In case of fire: Explosion risk. Evacuate area. DO NOT fight fire when fire reaches explosives. P370+P376 (P370 + P376): In case of fire: Stop leak if safe to do so. P370+P378.0 (P370 + P378): In case of fire: Use... to extinguish. P370+P378[abc] (P370 + P378): In case of fire: Use [abc] to extinguish. P370+P380+P375 (P370 + P380 + P375): In case of fire: Evacuate area. Fight fire remotely due to the risk of explosion. P370+P380+P375+P378.0 (P370 + P380 + P375 + P378): In case of fire: Evacuate area. Fight fire remotely due to the risk of explosion. Use ... to extinguish. P370+P380+P375+P378[abc] (P370 + P380 + P375 + P378): In case of fire: Evacuate area. Fight fire remotely due to the risk of explosion. Use [abc] to extinguish. P371+P380+P375 (P371 + P380 + P375): In case of major fire and large quantities: Evacuate area. Fight fire remotely due to the risk of explosion. P401.0 (P401): Store in accordance with... . P401[abc] (P401): Store in accordance with [abc]. P402 (P402): Store in a dry place. P403 (P403): Store in a well-ventilated place. P404 (P404): Store in a closed container. P405 (P405): Store locked up. P406.0 (P406): Store in a corrosion-resistant/... container with a resistant inner liner. P406.1 (P406): Store in a corrosion-resistant container with a resistant inner liner. P406[abc] (P406): Store in a [abc] container with a resistant inner liner. P407 (P407): Maintain air gap between stacks or pallets. P410 (P410): Protect from sunlight. P411.0 (P411): Store at temperatures not exceeding $\ldots{ }^{\circ} \mathrm{C} /$ $\ldots{ }^{\circ}$ F. P411.1[abc] (P411): Store at temperatures not exceeding abc ${ }^{\circ} \mathrm{C}$. P411.2[abc] (P411): Store at tem-
peratures not exceeding [def] ${ }^{\circ} \mathrm{F}$. P412.0 (P412): Do not expose to temperatures exceeding $50^{\circ} \mathrm{C} / 122^{\circ} \mathrm{F}$. P412.1 (P412): Do not expose to temperatures exceeding $50^{\circ} \mathrm{C}$. P412.2 (P412): Do not expose to temperatures exceeding $122^{\circ} \mathrm{F}$. P413.0 (P413): Store bulk masses greater than $\ldots \mathrm{kg} / \ldots \mathrm{lbs}$ at temperatures not exceeding $\ldots{ }^{\circ} \mathrm{C} / \ldots{ }^{\circ} \mathrm{F}$. P413.1[abc][def] (P413): Store bulk masses greater than [abc] kg at temperatures not exceeding [def] ${ }^{\circ} \mathrm{C}$. P413.2[abc][def] (P413): Store bulk masses greater than [abc] lbs at temperatures not exceeding [def] ${ }^{\circ} \mathrm{F}$. P420 (P420): Store separately. P402+P404 (P402 + P404): Store in a dry place. Store in a closed container. P403+P233 (P403 + P233): Store in a well-ventilated place. Keep container tightly closed. P403+P235 (P403 + P235): Store in a well-ventilated place. Keep cool. P410+P403 (P410 + P403): Protect from sunlight. Store in a well-ventilated place. P410+P412.0 (P410 + P412): Protect from sunlight. Do no expose to temperatures exceeding $50^{\circ} \mathrm{C} / 122^{\circ} \mathrm{F}$. $\mathbf{P 4 1 0 + \mathrm { P } 4 1 2 . 1 \text { ( } \mathrm { P } 4 1 0 + \mathrm { P } 4 1 2 \text { ): Protect from sunlight. }}$ Do no expose to temperatures exceeding $50^{\circ} \mathrm{C} . \mathbf{P 4 1 0 + P 4 1 2 . 2 ~ ( P 4 1 0 + P 4 1 2 ) : ~ P r o t e c t ~ f r o m ~ s u n l i g h t . ~ D o ~ n o ~}$ expose to temperatures exceeding $122^{\circ} \mathrm{F}$. P501.0 (P501): Dispose of contents/container to ... P501.0[abc] (P501): Dispose of contents/container to [abc] P501.1[abc] (P501): Dispose of contents to [abc] P501.2[abc] (P501): Dispose of container to [abc] P502 (P502): Refer to manufacturer or supplier for information on recovery or recycling.

## List of Implemented R and S Phrases

R1, R2, R3, R4, R5, R6, R7, R8, R9, R10, R11, R12, R14, R15, R16, R17, R18, R19, R20, R21, R22, R23, R24, R25, R26, R27, R28, R29, R30, R31, R32, R33, R34, R35, R36, R37, R38, R39, R40, R41, R42, R43, R44, R45, R46, R48, R49, R50, R51, R52, R53, R54, R55, R56, R57, R58, R59, R60, R61, R62, R63, R64, R65, R66, R67, R68, R14/15, R15/29, R20/21, R20/22, R20/21/22, R21/22, R23/24, R23/25, R23/24/25, R24/25, R26/27, R26/28, R26/27/28, R27/28, R36/37, R36/38, R36/37/38, R37/38, R39/23, R39/24, R39/25, R39/23/24, R39/23/25, R39/24/25, R39/23/24/25, R39/26, R39/27, R39/28, R39/26/27, R39/26/28, R39/27/28, R39/26/27/28, R42/43, R48/20, R48/21, R48/22, R48/20/21, R48/20/22, R48/21/22, R48/20/21/22, R48/23, R48/24, R48/25, R48/23/24, R48/23/25, R48/24/25, R48/23/24/25, R50/53, R51/53, R52/53, R68/20, R68/21, R68/22, R68/20/21, R68/20/22, R68/21/22, R68/20/21/22

S1, S2, S3, S4, S5[abc], S6[abc], S7, S8, S9, S12, S13, S14[abc], S15, S16, S17, S18, S20, S21, S22, S23[abc], S23.0, S23.1, S23.2, S23.3, S23.4, S24, S25, S26, S27, S28[abc], S29, S30, S33, S35, S36, S37, S38, S39, S40[abc], S41, S42 S43.0[abc], S43.1[abc], S45, S46[abc], S47[abc], S48[abc], S49, S50[abc], S51, S52, S53, S56, S57, S59, S60, S61, S62[abc], S63, S64, S1/2, S3/7, S3/9/14[abc], S3/9/14/49[abc], S3/9/49[abc], S3/14[abc], S7/8, S7/9, S7/47[abc], S20/21, S24/25, S27/28[abc], S29/35, S29/56, S36/37, S36/37/39[abc], S36/39[abc], S37/39, S47/49[abc]

Danish Thanks to the extensive help of Rasmus Villemoes, the Danish phrases could be included. There were a couple of typos in the official documents: We changed 'bebølse' to 'beboelse', 'omgåænde' to 'omgående' and 'producentesn' to 'producenten'.

French Dominique Richard helped with the French phrases. Many thanks to him!
German I adapted the German R and S Phrases to the current ('new') spelling. Therefore, when writing a text in german and using rsphrase, you will get a warning ('Your current language setting is german, rsphrase only knows the current German spelling (ngerman) which therefore was used.').

Italian Italian phrases implemented by Lorenzo Vagnarelli. Thanks a lot.
Spanish Ignacio Fernández Galván sent me the Spanish phrases. Thanks a lot!

