interface for upright greek letters for use in chemistry

Clemens Niederberger

http://www.mychemistry.eu/forums/forum/chemgreek/

contact@mychemistry.eu

- $2 e^-$

$$2 \text{Na} + \text{Cl}_2 \rightarrow 2 \text{Na}^+ + 2 \text{Cl}^- + 2 e^-$$

Table of Contents

List of Tables

1. Introduction
2. Licence and Requirements
3. News
   3.1. Version 0.2
   3.2. Version 0.3
   3.3. Version 0.4
   3.4. Version 0.5
   3.5. Version 0.5
   3.6. Version 1.0
4. Define Mappings
5. Predefined Mappings and Selection of a Mapping
6. Changing a Specific Symbol in an Existing Mapping
7. Inspecting a Mapping

8. Additional Macros
   8.1. Overview Over the Mappings
   8.2. Mapping ‘default’
   8.3. Mapping ‘var-default’
   8.4. Mapping ‘upgreek’
   8.5. Mapping ‘newtx’
   8.6. Mapping ‘kpfonts’
   8.7. Mapping ‘pxgreeks’
   8.8. Mapping ‘mathdesign’ with package option ‘utopia’
   8.9. Mapping ‘mathdesign’ with package option ‘charter’
   8.10. Mapping ‘fourier’
   8.11. Mapping ‘textalpha’
   8.12. Mapping ‘fontspec’ with ‘Linux Libertine’

9. References
10. Index
List of Tables

1. Predefined mappings ........................................ 6
2. A demonstration of the \printchemgreekmapping command .... 8

1. Introduction

The \texttt{chemgreek} package is an auxiliary package for other chemistry packages such as chem-macros. In chemistry there is often the need for upright greek letters. The \texttt{chemgreek} package provides an interface to various other packages that provide upright greek letters. One could mention \texttt{textgreek}, \texttt{upgreek}, \texttt{newtx} or \texttt{kpfonts}. All of these packages provide upright greek letters, some a whole alphabet some only the upright variants of the standard italic symbols for which macros are defined in base \LaTeX.

\texttt{chemgreek} offers a possibility to map those different interfaces to a unified set of macros for usage in a chemistry package. This is useful as then for example names like $\beta$-d-glucopyranose can be typeset with a semantic interface and still have matching greek letters while the user is not limited to a certain package or font. Consequently this package is used by the chemmacros package \cite{Nie15a} and its \texttt{iupac} naming commands, for example, and by the chemnum package \cite{Nie15b}.

2. Licence and Requirements

Permission is granted to copy, distribute and/or modify this software under the terms of the \LaTeX Project Public License (\texttt{LPPL}), version 1.3 or later (http://www.latex-project.org/lppl.txt). The software has the status “maintained.”

\texttt{chemgreek} loads the following packages: \texttt{expl3} \cite{L3Pa}, \texttt{xparse} \cite{L3Pb} and \texttt{amstext} \cite{MS00}.

3. News

3.1. Version 0.2

- The mapping “mathdesign” has been added. In order to use it you need the mathdesign package \cite{Pic13} loaded and use one of its options.

- The mapping “fourier” has been added. In order to use it you need the fourier package \cite{Bov05} loaded.

3.2. Version 0.3

- The provided macros have been renamed from \texttt{Chem(...)} into \texttt{chem(...)}. The uppercase version still are provided for backwards compatibility but issue a warning message and

\footnotesize

1. on ctan as \texttt{l3kernel}: \url{http://mirrors.ctan.org/macros/latex/contrib/l3kernel/}
2. on ctan as \texttt{l3packages}: \url{http://mirrors.ctan.org/macros/latex/contrib/l3packages/}
3. \url{http://ctan.org/tex-archive/macros/latex/required/amslatex/math}
3. News

will be removed some time in the future.

• The commands for defining mappings have gotten an optional argument which allows to specify the name of the package a mapping needs. The command \selectchemgreekmapping now checks for this package and gives a warning if it doesn’t find it loaded.

• The mapping “textalpha” has been added. In order to use it you need the textalpha package (part of greek-fontenc [Mil13]) loaded.

• If the package hyperref [OR12] is loaded with the unicode option and the textalpha package has been loaded at begin document all the \chem(... commands are let to textalpha’s \text(...) commands for the PDF bookmarks. This allows Greek letters in the bookmarks without worrying about \texorpdfstring.

3.3. Version 0.4

• The mapping “fontspec” has been added. In order to use it you need the fontspec package [RH13] loaded. This means it can only be used with Lua\TeX or Xe\TeX.

• New command \printchemgreekalphabet.

3.4. Version 0.5

• The package is now distributed independently from the chemmacros package.

3.5. Version 0.5

• The deprecated macros \Chem(...) have been dropped and will now cause an error if used.

3.6. Version 1.0

• If a mapping is activated that needs a package and the package is missing \CHEMGREEK falls back to the ‘default’ mapping now.

• If exactly one package for one of the mappings has been loaded the corresponding mapping is activated at begin document, see also section 5.

• expl3 versions of the letter macros (\chemgreek_alpha:, \chemgreek_Alpha:, ...)

• New macros \chemgreekmappingsymbol (see section 8), \newchemgreekmappingalias, \renewchemgreekmappingalias and \declarechemgreekmappingalias (see section 4).
4. Define Mappings

\texttt{CHEMGREEK}'s main commands are:

\textbf{\texttt{\textbackslash newchemgreekmapping}(\texttt{\{package\}}\texttt{\{name\}}\texttt{\{mapping list\})}}

Add a new mapping to \texttt{CHEMGREEK}. Issues an error if a mapping with the same name already exists. With the optional argument the package that is needed for this mapping can (and should) be specified.

\textbf{\texttt{\textbackslash renewchemgreekmapping}(\texttt{\{package\}}\texttt{\{name\}}\texttt{\{mapping list\})}}

Renew a \texttt{CHEMGREEK} mapping. Issues an error if the mapping doesn’t exist yet. With the optional argument the package that is needed for this mapping can (and should) be specified.

\textbf{\texttt{\textbackslash declarechemgreekmapping}(\texttt{\{package\}}\texttt{\{name\}}\texttt{\{mapping list\})}}

Declare a new mapping to \texttt{CHEMGREEK}. If the mapping already exists it will be overwritten. With the optional argument the package that is needed for this mapping can (and should) be specified.

\textbf{\texttt{\textbackslash newchemgreekmappingalias}(\texttt{\{new mapping name\}}\texttt{\{existing mapping name\})}}

Define an alias mapping. Issues an error if \texttt{\{new mapping name\}} already exists.

\textbf{\texttt{\textbackslash renewchemgreekmappingalias}(\texttt{\{new mapping name\}}\texttt{\{existing mapping name\})}}

Redeﬁne a mapping to an alias of an existing mapping. Issues an error if \texttt{\{new mapping name\}} doesn’t exist, yet.

\textbf{\texttt{\textbackslash declarechemgreekmappingalias}(\texttt{\{new mapping name\}}\texttt{\{existing mapping name\})}}

Define an alias mapping. Doesn’t check, if \texttt{\{new mapping name\}} exists or not.

The command \texttt{\textbackslash newchemgreekmapping} needs to get a comma separated list of 24 pairs divided by a slash. The ﬁrst entry is the lowercase version und the second the uppercase version for the corresponding greek letter at the current position. This will become clearer if you look at how the default mapping is deﬁned:

```
\newchemgreekmapping{default}
{
\ensuremath{\alpha} / \ensuremath{\mathrm{A}} , % 1: alpha
\ensuremath{\beta} / \ensuremath{\mathrm{B}} , % 2: beta
\ensuremath{\gamma} / \ensuremath{\Gamma} , % 3: gamma
\ensuremath{\delta} / \ensuremath{\Delta} , % 4: delta
\ensuremath{\epsilon} / \ensuremath{\mathrm{E}} , % 5: epsilon
\ensuremath{\zeta} / \ensuremath{\mathrm{Z}} , % 6: zeta
\ensuremath{\eta} / \ensuremath{\mathrm{H}} , % 7: eta
\ensuremath{\theta} / \ensuremath{\Theta} , % 8: theta
\ensuremath{\iota} / \ensuremath{\mathrm{I}} , % 9: iota
\ensuremath{\kappa} / \ensuremath{\mathrm{K}} , % 10: kappa
\ensuremath{\lambda} / \ensuremath{\Lambda} , % 11: lambda
\ensuremath{\mu} / \ensuremath{\mathrm{M}} , % 12: mu
```

5. Predefined Mappings and Selection of a Mapping

There must be 24 pairs of entries, i.e., a complete mapping! Those entries are the ones that will be used by the interface macros. For each letter a pair \chemalpha/chemAlpha is defined that uses the entries of the currently active mapping. That means there are 48 (robust) macros defined each beginning with \chem... followed by the lowercase or uppercase name of the Greek letter.

The default mapping is – as you can probably see – not an upright one. This is because \chemgreek will not make any choice for a specific package but lets the user (or another package) choose. \chemgreek however recognizes if an unambiguous choice for one of the upright mappings is possible and if it is will select the appropriate mapping at begin document.

\l_chemgreek_active_mapping_tl
The currently active mapping is always available in the token list variable.

5. Predefined Mappings and Selection of a Mapping

\chemgreek predefines some mappings. Some of the mappings require additional packages to be loaded. The mapping names and the required packages are listed in table 1. The mapping fontspec is a bit different here: if you use this mapping then the fact is used that fontspec also defines commands like \textalpha. However, they only work if you also use a font that has the Greek glyphs.

If exactly one of the packages required by one of the mappings has been loaded such that an unambiguous choice is possible then \chemgreek will choose and activate the corresponding
5. Predefined Mappings and Selection of a Mapping

<table>
<thead>
<tr>
<th>mapping</th>
<th>package</th>
</tr>
</thead>
<tbody>
<tr>
<td>default</td>
<td>—</td>
</tr>
<tr>
<td>var-default</td>
<td>—</td>
</tr>
<tr>
<td>textgreek</td>
<td>textgreek [Mic11]</td>
</tr>
<tr>
<td>upgreek</td>
<td>upgreek [Scho3]</td>
</tr>
<tr>
<td>newtx</td>
<td>newtxmath [Sha13]</td>
</tr>
<tr>
<td>kpfonts</td>
<td>kpfonts [Cai10]</td>
</tr>
<tr>
<td>pxgreesks</td>
<td>pxgreesks [Bur11]</td>
</tr>
<tr>
<td>mathdesign</td>
<td>mathdesign [Pic13]</td>
</tr>
<tr>
<td>fourier</td>
<td>fourier [Bov05]</td>
</tr>
<tr>
<td>textalpha</td>
<td>textalpha [Mil13]</td>
</tr>
<tr>
<td>fontscl</td>
<td>fontscl [RH13]</td>
</tr>
</tbody>
</table>

Table 1: Predefined mappings.

A mapping is selected and activated manually with one of the following commands:

\activatechemgreekmapping*{(⟨name⟩)}

This command selects and activates the mapping ⟨name⟩. If the star variant is used also the package of mapping ⟨name⟩ (as defined with \newchemgreekmapping) is loaded. Otherwise a required package has to be loaded additionally the usual way via \usepackage or \RequirePackage. If the package hasn’t been loaded a warning will be written to the log and the ‘default’ mapping will be activated instead. *The command can only be used in the document preamble.*

\selectchemgreekmapping{(⟨name⟩)}

This command selects and activates the mapping ⟨name⟩. A required package has to be loaded additionally the usual way via \usepackage or \RequirePackage. If the package hasn’t been loaded a warning will be written to the log and the ‘default’ mapping will be activated instead. *The command can be used throughout the document.*

\chemphi\ and \chemPhi, \$\phi\$ and \$\Phi\$

\selectchemgreekmapping(newtx)

\chemphi\ and \chemPhi, \$\phi\$ and \$\Phi\$

ϕ and Φ, ϕ and Φ
Since the fontspec mapping is a little bit different than the others I’d like to show a little example for it. The difference is subtle: you need to choose a font containing the needed glyphs.

\begin{verbatim}
\documentclass[margin=3pt]{standalone}
\usepackage{fontspec}
\setmainfont{LinLibertine_R.otf}\% need a font that has the glyphs!
\usepackage{chemgreek}
\selectchemgreekmapping{fontspec}
\begin{document}
\printchemgreekalphabet
\end{document}
\end{verbatim}

6. Changing a Specific Symbol in an Existing Mapping

If you should want to change a specific entry of a specific mapping it would be rather tedious to redefine the whole mapping. That is why \texttt{chemgreek} provides a command for that purpose:

\begin{verbatim}
\changechemgreeksymbol{{mapping name}}{upper|lower}{{entry name}}{⟨entry⟩}
\end{verbatim}

Changes the upper- or lowercase entry \texttt{⟨entry name⟩} in the mapping \texttt{⟨mapping name⟩}.

In order to activate the change you need the (re-) activate the affected mapping afterwards:

\begin{verbatim}
\chemalpha
\changechemgreeksymbol{default}{lower}{alpha}{xxx}\
\selectchemgreekmapping{default}
\chemalpha
\end{verbatim}

7. Inspecting a Mapping

If you want to check if a mapping has been correctly set you can use the following commands:

\begin{verbatim}
\printchemgreekmapping{⟨mapping⟩}
\end{verbatim}

This will typeset a table (using a simple \texttt{tabular} environment) with all 48 characters like the one shown in table 2.
### 8. Additional Macros

<table>
<thead>
<tr>
<th>pos</th>
<th>name</th>
<th>lower</th>
<th>upper</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>alpha</td>
<td>α</td>
<td>A</td>
</tr>
<tr>
<td>2.</td>
<td>beta</td>
<td>β</td>
<td>B</td>
</tr>
<tr>
<td>3.</td>
<td>gamma</td>
<td>γ</td>
<td>Γ</td>
</tr>
<tr>
<td>4.</td>
<td>delta</td>
<td>δ</td>
<td>Δ</td>
</tr>
<tr>
<td>5.</td>
<td>epsilon</td>
<td>ε</td>
<td>E</td>
</tr>
<tr>
<td>6.</td>
<td>zeta</td>
<td>ζ</td>
<td>Z</td>
</tr>
<tr>
<td>7.</td>
<td>eta</td>
<td>η</td>
<td>H</td>
</tr>
<tr>
<td>8.</td>
<td>theta</td>
<td>θ</td>
<td>Θ</td>
</tr>
<tr>
<td>9.</td>
<td>iota</td>
<td>ι</td>
<td>I</td>
</tr>
<tr>
<td>10.</td>
<td>kappa</td>
<td>κ</td>
<td>K</td>
</tr>
<tr>
<td>11.</td>
<td>lambda</td>
<td>λ</td>
<td>Λ</td>
</tr>
<tr>
<td>12.</td>
<td>mu</td>
<td>µ</td>
<td>M</td>
</tr>
<tr>
<td>13.</td>
<td>nu</td>
<td>ν</td>
<td>N</td>
</tr>
<tr>
<td>14.</td>
<td>xi</td>
<td>ξ</td>
<td>Ξ</td>
</tr>
<tr>
<td>15.</td>
<td>omikron</td>
<td>o</td>
<td>O</td>
</tr>
<tr>
<td>16.</td>
<td>pi</td>
<td>π</td>
<td>Π</td>
</tr>
<tr>
<td>17.</td>
<td>rho</td>
<td>ρ</td>
<td>R</td>
</tr>
<tr>
<td>18.</td>
<td>sigma</td>
<td>σ</td>
<td>Σ</td>
</tr>
<tr>
<td>19.</td>
<td>tau</td>
<td>τ</td>
<td>T</td>
</tr>
<tr>
<td>20.</td>
<td>upsilon</td>
<td>υ</td>
<td>Y</td>
</tr>
<tr>
<td>21.</td>
<td>phi</td>
<td>ϕ</td>
<td>Φ</td>
</tr>
<tr>
<td>22.</td>
<td>chi</td>
<td>χ</td>
<td>Χ</td>
</tr>
<tr>
<td>23.</td>
<td>psi</td>
<td>ψ</td>
<td>Ψ</td>
</tr>
<tr>
<td>24.</td>
<td>omega</td>
<td>ω</td>
<td>Ω</td>
</tr>
</tbody>
</table>

**Table 2:** A demonstration of the \printchemgreekmapping command.

\printchemgreekalphabet

Introduced in version 0.4

This will print the twentyfour pairs of lower- and uppercase letters of the currently active mapping: \(\alpha\A, \beta\B, \gamma\Gamma, \delta\Delta, \epsilon\E, \zeta\Z, \eta\H, \theta\Theta, \iota\I, \kappa\K, \lambda\Lambda, \mu\M, \nu\N, \xi\Xi, \omicron\O, \pi\Pi, \rho\R, \sigma\Sigma, \tau\T, \upsilon\U, \phi\Phi, \chi\X, \psi\Psi, \omega\Omega.

\showchemgreekmapping{(mapping)}

Changed in version 0.3

This command will write information about the definition of all 48 macros for a mapping to the log file.

### 8. Additional Macros

\chemgreekmappingsymbol{(mapping name)}{(symbol name)}

A command which prints a specific symbol of a specific mapping. The mapping (mapping name) doesn’t need to be active but package dependencies must be taken care of, *i.e.*, if (mapping name) needs a certain package to be loaded you should make sure that it is.
A. Overviews Over the Mappings

A.1. Mapping ‘default’
\[\alpha \beta \gamma \delta \epsilon \zeta \eta \theta \iota \kappa \lambda \mu \nu \xi \omicron \pi \rho \sigma \tau \upsilon \phi \chi \psi \omega\]

A.2. Mapping ‘var-default’
\[\alpha \beta \gamma \delta \epsilon \zeta \eta \theta \iota \kappa \lambda \mu \nu \xi \omicron \pi \rho \zeta \tau \upsilon \phi \chi \psi \omega\]

A.3. Mapping ‘textgreek’
\[\alpha \beta \gamma \delta \epsilon \zeta \eta \theta \iota \kappa \lambda \mu \nu \xi \omicron \pi \tau \upsilon \phi \chi \psi \omega\]

A.4. Mapping ‘upgreek’
\[\alpha \beta \gamma \delta \epsilon \zeta \eta \theta \iota \kappa \lambda \mu \nu \xi \omicron \pi \tau \upsilon \phi \chi \psi \omega\]

A.5. Mapping ‘newtx’
\[\alpha \beta \gamma \delta \epsilon \zeta \eta \theta \iota \kappa \lambda \mu \nu \xi \omicron \pi \rho \sigma \tau \upsilon \phi \chi \psi \omega\]

A.6. Mapping ‘kpfonts’
\[\alpha \beta \gamma \delta \epsilon \zeta \eta \theta \iota \kappa \lambda \mu \nu \xi \omicron \pi \rho \sigma \tau \upsilon \phi \chi \psi \omega\]

A.7. Mapping ‘pxgreesks’
\[\alpha \beta \gamma \delta \epsilon \zeta \eta \theta \iota \kappa \lambda \mu \nu \xi \omicron \pi \rho \sigma \tau \upsilon \phi \chi \psi \omega\]

A.8. Mapping ‘mathdesign’ with package option \texttt{utopia}
\[\alpha \beta \gamma \delta \epsilon \zeta \eta \theta \iota \kappa \lambda \mu \nu \xi \omicron \pi \rho \sigma \tau \upsilon \phi \chi \psi \omega\]

A.9. Mapping ‘mathdesign’ with package option \texttt{charter}
\[\alpha \beta \gamma \delta \epsilon \zeta \eta \theta \iota \kappa \lambda \mu \nu \xi \omicron \pi \rho \sigma \tau \upsilon \phi \chi \psi \omega\]

A.10. Mapping ‘fourier’
\[\alpha \beta \gamma \delta \epsilon \zeta \eta \theta \iota \kappa \lambda \mu \nu \xi \omicron \pi \rho \sigma \tau \upsilon \phi \chi \psi \omega\]
A.11. Mapping ‘textalpha’
\[\alpha \beta \gamma \delta \varepsilon \zeta \eta \theta \iota \kappa \lambda \mu \nu \Xi \omicron \pi \rho \sigma \tau \upsilon \phi \chi \psi \Omega\]

A.12. Mapping ‘fontspec’ with Font ‘Linux Libertine’
\[\alpha \beta \gamma \delta \varepsilon \zeta \eta \theta \iota \kappa \lambda \mu \nu \Xi \omicron \pi \rho \sigma \tau \upsilon \phi \chi \psi \Omega\]

B. References

url: http://mirror.ctan.org/fonts/fourier-.gut/.

url: http://mirror.ctan.org/macros/latex/contrib/pxgreeks/.


url: http://mirror.ctan.org/macros/latex/contrib/l3kernel/.

[L3Pb] The \LaTeX{}3 Project Team. l3packages. version SVN 6377, Jan. 19, 2016.
url: http://mirror.ctan.org/macros/latex/contrib/l3packages/.

url: http://mirror.ctan.org/macros/latex/contrib/textgreek/.


[MSoo] Frank MITTELBACH and Rainer SCHÖPF. amstext. version 2.01, June 29, 2000.
url: http://mirror.ctan.org/macros/latex/required/amstext/.

url: http://mirror.ctan.org/macros/latex/contrib/chemmacros/.

url: http://mirror.ctan.org/macros/latex/contrib/chemnum/.

url: http://mirror.ctan.org/macros/latex/contrib/hyperref/.

url: http://mirror.ctan.org/fonts/mathdesign/.

url: http://mirror.ctan.org/macros/latex/contrib/fontspec/.

url: http://mirror.ctan.org/macros/latex/contrib/was/.

url: http://mirror.ctan.org/fonts/newtx/.
## C. Index

| A | \activatechemgreekmapping ........................................ 6  |
|   | amstext (package) .............................................. 2  |
| B | Bovani, Michel .................................................. 2, 6  |
|   | Burnol, Jean-François .......................................... 6  |
| C | Caignaert, Christophe .......................................... 6  |
|   | \changechemgreeksymbol ........................................ 7  |
|   | \chemAlpha .......................................................... 5  |
|   | \chemalpha .......................................................... 5  |
|   | \chemgreekmappingsymbol ....................................... 3, 8  |
|   | chemnum (package) ................................................. 2  |
|   | \chemPhi ............................................................ 4  |
|   | \chemphi ............................................................ 5  |
| CTAN | .............................................................. 2  |
| D | \declarechemgreekmapping ....................................... 4  |
|   | \declarechemgreekmappingalias .................................. 3  |
| E | expl3 (package) ................................................... 2  |
| F | fontspec (package) ................................................. 3, 5  |
|   | fourier (package) ................................................ 6  |
| G | greek-fontenc (bundle) .......................................... 3, 6  |
| H | Hosny, Khaled ...................................................... 3, 6  |
|   | hyperref (package) ............................................... 3  |
| K | kpfonts (package) ................................................ 2, 6  |
| L | \lmodernkernel (bundle) .......................................... 2  |
|   | \lmodernpackages (bundle) ....................................... 2  |
|   | \_chemgreek_active_mapping_tl .................................. 5  |
|   | LPPL ................................................................. 2  |
| M | mathdesign (package) ............................................ 2, 6  |
|   | Michlmayr, Leonard .............................................. 6  |
|   | Milde, Günter .................................................... 3, 6  |
|   | Mittelbach, Frank ............................................... 2  |
| N | Niederberger, Clemens ........................................... 2  |
| O | Oberdiek, Heiko .................................................. 3  |
| P | Pichaud, Paul ..................................................... 2, 6  |
|   | \printchemgreekalphabet ........................................ 3, 7  |
|   | \printchemgreekmapping ......................................... 7  |
|   | pxgreek (package) ................................................ 6  |
| R | Rahtz, Sebastian ................................................ 3  |
|   | \renewchemgreekmapping ......................................... 4  |
|   | \renewchemgreekmappingalias .................................... 3  |
|   | Robertson, Will ................................................... 3, 6  |
| S | Schöpf, Rainer ................................................... 2  |
|   | Schmidt, Walter .................................................... 6  |
|   | \selectchemgreekmapping ........................................ 3, 6  |
|   | Sharpe, Michael ................................................... 6  |
|   | \showchemgreekmapping .......................................... 8  |
| T | textalpha (package) .............................................. 3, 6  |
|   | textgreek (package) .............................................. 2, 6  |
|   | The \LaTeX{} Project Team ....................................... 2  |
| U | upgreek (package) ............................................... 2, 6  |
| X | xparse (package) ................................................. 2  |