CHEMGREEK

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interface for upright greek letters for use in chemistry

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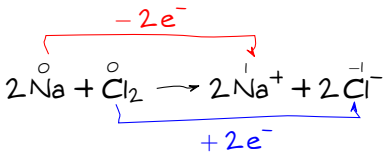

Table of Contents

List of Tables 2

1. Introduction 2

2. Licence and Requirements 2

3. News 2
   - 3.1. Version 0.2 . . . 2
   - 3.2. Version 0.3 . . . 2
   - 3.3. Version 0.4 . . . 3
   - 3.4. Version 0.5 . . . 3
   - 3.5. Version 0.5 . . . 3
   - 3.6. Version 1.0 . . . 3

4. Define Mappings 4

5. Predefined Mappings and Selection of a Mapping 5

6. Changing a Specific Symbol in an Existing Mapping 7

7. Inspecting a Mapping 7

8. Additional Macros 8

A. Overviews Over the Mappings 9
   - A.1. Mapping ‘default’ . . . 9
   - A.2. Mapping ‘var-default’ . . . 9
   - A.3. Mapping ‘textgreek’ . . . 9
   - A.4. Mapping ‘upgreek’ . . . 9
   - A.5. Mapping ‘newtx’ . . . 9
   - A.6. Mapping ‘kpfonts’ . . . 9
   - A.7. Mapping ‘pxgreeks’ . . . 9
   - A.8. Mapping ‘mathdesign’ with package option utopia . . . 9
   - A.9. Mapping ‘mathdesign’ with package option charter . . . 9
   - A.10. Mapping ‘fourier’ . . . 9
   - A.11. Mapping ‘textalpha’ . . . 10
   - A.12. Mapping ‘fontspec’ with Font ‘Linux Libertine’ . . . 10

B. References 10

C. Index 11

List of Tables

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

1. Introduction

The CHEMGREEK package is an auxiliary package for other chemistry packages such as chemmacros. In chemistry there is often the need for upright greek letters. The CHEMGREEK package provides an interface to various other packages that provide upright greek letters. One could mention textgreek, upgreek, newtx or 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.

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 β-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 [Nie19] and its IUPAC naming commands, for example, and by the chemnum package [Nie16].

2. Licence and Requirements

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

CHEMGREEK loads the following packages: expl3 [1] [L3Pa], xparse [2] [L3Pb] and amstext [3] [MSoo].

3. News

3.1. Version 0.2

- The mapping "mathdesign" has been added. In order to use it you need the mathdesign package [Pic13] loaded and use one of its options.
- The mapping "fourier" has been added. In order to use it you need the fourier package [Bovo5] loaded.

3.2. Version 0.3

- The provided macros have been renamed from \Chem⟨...⟩ into \chem⟨...⟩. The uppercase version still are provided for backwards compatibility but issue a warning message and

1. on CTAN as l3kernel: http://mirrors.ctan.org/macros/latex/contrib/l3kernel/
2. on CTAN as l3packages: http://mirrors.ctan.org/macros/latex/contrib/l3packages/
3. http://ctan.org/tex-archive/macros/latex/required/amslatex/math

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 [Mil19]) loaded.
- If the package hyperref [OR19] 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 [RH19] loaded. This means it can only be used with LuaLaTeX or XeLaTeX.
- 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

CHEMGREEK's main commands are:

`\newchemgreekmapping[`⟨*package*⟩`]{`⟨*name*⟩`}{`⟨*mapping list*⟩`}`

Changed in version 0.3

Add a new mapping to 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.

`\renewchemgreekmapping[`⟨*package*⟩`]{`⟨*name*⟩`}{`⟨*mapping list*⟩`}`

Changed in version 0.3

Renew a 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.

`\declarechemgreekmapping[`⟨*package*⟩`]{`⟨*name*⟩`}{`⟨*mapping list*⟩`}`

Changed in version 0.3

Declare a new mapping to 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.

`\newchemgreekmappingalias{`⟨*new mapping name*⟩`}{`⟨*existing mapping name*⟩`}`

Introduced in version 1.0

Define an alias mapping. Issues an error if ⟨*new mapping name*⟩ already exists.

`\renewchemgreekmappingalias{`⟨*new mapping name*⟩`}{`⟨*existing mapping name*⟩`}`

Introduced in version 1.0

Redefine a mapping to an alias of an existing mapping. Issues an error if ⟨*new mapping name*⟩ doesn't exist, yet.

`\declarechemgreekmappingalias{`⟨*new mapping name*⟩`}{`⟨*existing mapping name*⟩`}`

Introduced in version 1.0

Define an alias mapping. Doesn't check, if `{`⟨*new mapping name*⟩`}` exists or not.

The command `\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
```

```
    \ensuremath{\nu}      / \ensuremath{\mathrm{N}} , % 13: nu
    \ensuremath{\xi}      / \ensuremath{\Xi} ,        % 14: xi
    \ensuremath{o}        / \ensuremath{\mathrm{O}} , % 15: omikron
    \ensuremath{\pi}      / \ensuremath{\Pi} ,        % 16: pi
    \ensuremath{\rho}     / \ensuremath{\mathrm{P}} , % 17: rho
    \ensuremath{\sigma}   / \ensuremath{\Sigma} ,     % 18: sigma
    \ensuremath{\tau}     / \ensuremath{\mathrm{T}} , % 19: tau
    \ensuremath{\upsilon} / \ensuremath{\Upsilon} ,   % 20: upsilon
    \ensuremath{\phi}     / \ensuremath{\Phi} ,       % 21: phi
    \ensuremath{\psi}     / \ensuremath{\Psi} ,       % 22: psi
    \ensuremath{\chi}     / \ensuremath{\mathrm{X}} , % 23: chi
    \ensuremath{\omega}   / \ensuremath{\Omega}       % 24: omega
}
```

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.

```
Default mapping: \chemphi\ and \chemPhi, $\phi$ and $\Phi$
```

Default mapping: ϕ and Φ, ϕ and Φ

\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

mapping	package
default	—
var-default	—
textgreek	textgreek [Mic11]
upgreek	upgreek [Sch03]
newtx	newtxmath [Sha18]
kpfonts	kpfonts [Cai18]
pxgreeks	pxgreeks [Bur11]
mathdesign	mathdesign [Pic13]
fourier	fourier [Bov05]
textalpha	textalpha [Mil19]
fontspec	fontspec [RH19]

Table 1: Predefined mappings.

mapping at begin document. If an umbiguous choice isn't possible then CHEMGREEK will select the 'default' mapping at begin document. If a user has selected a mapping manually in the preamble (with one of the commands explained in a bit) then CHEMGREEK will do nothing on its own.

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

`\activatechemgreekmapping*{`⟨*name*⟩`}`

Changed in version 1.0

This commands 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*⟩`}`

Changed in version 1.0

This commands 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.*

```
% requires the `newtxmath' package to be loaded:
\chemphi\ and \chemPhi, $\phi$ and $\Phi$\par
\selectchemgreekmapping{newtx}
\chemphi\ and \chemPhi, $\upphi$ and $\upPhi$
```

ϕ and Φ, ϕ and Φ

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.

```
\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}
```

αA βB γΓ δΔ εE ζZ ηH θΘ ιI κK λΛ μM νN ξΞ oO πΠ ρP σΣ τT υY φΦ χX ψΨ ωΩ

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 CHEMGREEK provides a command for that purpose:

`\changechemgreeksymbol{`⟨*mapping name*⟩`}{upper|lower}{`⟨*entry name*⟩`}{`⟨*entry*⟩`}`
Changes the `upper`- or `lower`case entry ⟨*entry name*⟩ in the mapping ⟨*mapping name*⟩.

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

```
\chemalpha
\changechemgreeksymbol{default}{lower}{alpha}{xxx}%
\selectchemgreekmapping{default}
\chemalpha
```

α xxx

7. Inspecting a Mapping

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

`\printchemgreekmapping{`⟨*mapping*⟩`}`
Introduced in version 0.3
This will typeset a table (using a simple `tabular` environment) with all 48 characters like the one shown in table 2.

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

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: αA βB γΓ δΔ ϵE ζZ ηH θΘ ιI κK λΛ μM νN ξΞ οO πΠ ρR σΣ τT υϒ ϕΦ χX ψΨ ωΩ.

`\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’

αA βB $\gamma\Gamma$ $\delta\Delta$ ϵE ζZ ηH $\theta\Theta$ ιI κK $\lambda\Lambda$ μM νN $\xi\Xi$ oO $\pi\Pi$ ρP $\sigma\Sigma$ τT $\upsilon\Upsilon$ $\phi\Phi$ χX $\psi\Psi$ $\omega\Omega$

A.2. Mapping ‘var-default’

αA βB $\gamma\Gamma$ $\delta\Delta$ εE ζZ ηH $\vartheta\Theta$ ιI κK $\lambda\Lambda$ μM νN $\xi\Xi$ oO $\varpi\Pi$ ϱP $\varsigma\Sigma$ τT $\upsilon\Upsilon$ $\varphi\Phi$ χX $\psi\Psi$ $\omega\Omega$

A.3. Mapping ‘textgreek’

αA βB γΓ δΔ εE ζZ ηH ϑΘ ιI κK λΛ μM νN ξΞ oO πΠ ρP σΣ τT υϒ φΦ χX ψΨ ωΩ

A.4. Mapping ‘upgreek’

αA βB γΓ δΔ εE ζZ ηH θΘ ιI κK λΛ μM νN ξΞ oO πΠ ρR σΣ τT υϒ ϕΦ χX ψΨ ωΩ

A.5. Mapping ‘newtx’

αA βB γΓ δΔ εE ζZ ηH θΘ ιI κK λΛ μM νN ξΞ oO πΠ ρR σΣ τT υϒ ϕΦ χX ψΨ ωΩ

A.6. Mapping ‘kpfonts’

αA βB γΓ δΔ εE ζZ ηH θΘ ιI κK λΛ μM νN ξΞ oO πΠ ρR σΣ τT υϒ ϕΦ χX ψΨ ωΩ

A.7. Mapping ‘pxgreeks’

αA βB γΓ δΔ εE ζZ ηH θΘ ιI κK λΛ μM νN ξΞ oO πΠ ρR σΣ τT υϒ ϕΦ χX ψΨ ωΩ

A.8. Mapping ‘mathdesign’ with package option utopia

αA βB γΓ δΔ εE ζZ ηH θΘ ιI κK λΛ μM νN ξΞ oO πΠ ρR σΣ τT υϒ ϕΦ χX ψΨ ωΩ

A.9. Mapping ‘mathdesign’ with package option charter

αA βB γΓ δΔ εE ζZ ηH θΘ ιI κK λΛ μM νN ξΞ oO πΠ ρR σΣ τT υϒ ϕΦ χX ψΨ ωΩ

A.10. Mapping ‘fourier’

αA βB γΓ δΔ εE ζZ ηH θΘ ιI κK λΛ μM νN ξΞ oO πΠ ρR σΣ τT υϒ ϕΦ χX ψΨ ωΩ

A.11. Mapping ‘textalpha’

αA βB γΓ δΔ εE ζZ ηH ϑΘ ιI κK λΛ μM νN ξΞ οO πΠ ρP σΣ τT υϒ φΦ χX ψΨ ωΩ

A.12. Mapping ‘fontspec’ with Font ‘Linux Libertine’

αA βB γΓ δΔ εE ζZ ηH θΘ ιI κK λΛ μM νN ξΞ οO πΠ ρP σΣ τT υY φΦ χX ψΨ ωΩ

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C. Index

A

\activatechemgreekmapping 6
amstext 2
amstext (package) 2

B

Bovani, Michel 2, 6
Burnol, Jean-François 6

C

Caignaert, Christophe 6
\changechemgreeksymbol 7
\chemAlpha 5
\chemalpha 5, 7
\chemgreekmappingsymbol 3, 8
chemmacros 2
chemmacros (package) . . . . . 2 f.
chemnum 2
chemnum (package) 2
\chemPhi . . . . . 5 f.
\chemphi . . . . . 5 f.
ctan 2

D

\declarechemgreekmapping 4
\declarechemgreekmappingalias . . . . . 3 f.

E

expl3 (package) 2

F

fontspec 3, 6
fontspec (package) . . . . . 3, 5 f.
fourier 2, 6
fourier (package) 2, 6

G

greek-fontenc 3, 6
greek-fontenc (bundle) 3

H

Hosny, Khaled 3, 6
hyperref 3
hyperref (package) 3

K

kpfonts 6
kpfonts (package) 2, 6

L

l3kernel 2
l3packages 2
\l_chemgreek_active_mapping_tl 5
lppl 2

M

mathdesign 2, 6
mathdesign (package) 2, 6
Michlmayr, Leonard 6
Milde, Günter 3, 6
Mittelbach, Frank 2

N

\newchemgreekmapping 4, 6
\newchemgreekmappingalias . . . . . 3 f.
newtx 6
newtx (package) 2
Niederberger, Clemens 2

O

Oberdiek, Heiko 3

P

Pichaureau, Paul 2, 6
\printchemgreekalphabet . . . . . 3, 7 f.
\printchemgreekmapping 7
pxgreeks 6
pxgreeks (package) 6

R

Rahtz, Sebastian 3
\renewchemgreekmapping 4
\renewchemgreekmappingalias . . . . . 3 f.
Robertson, Will 3, 6

S

Schmidt, Walter 6

Schöpf, Rainer 2
\selectchemgreekmapping . . . . . 3, 6 f.
Sharpe, Michael 6
\showchemgreekmapping 8

T
textalpha (package) 3, 6
textgreek 6
textgreek (package) 2, 6
The LaTeX3 Project Team 2

U
upgreek 6
upgreek (package) 2, 6

X
xparse (package) 2