

CHEMGREEK

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interface for upright greek letters for use in chemistry

Clemens NIEDERBERGER

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

contact@mychemistry.eu

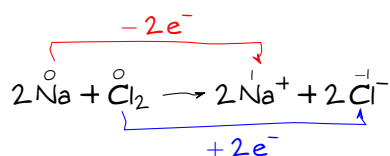


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1. Introduction

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 L^AT_EX.

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 [Nie15a] and its IUPAC naming commands, for example, and by the chemnum package [Nie15b].

2. Licence and Requirements

Permission is granted to copy, distribute and/or modify this software under the terms of the L^AT_EX 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: expl3¹ [L3Pa], xparse² [L3Pb] and amstext³ [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>

4. Define Mappings

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 \LaTeX or Xe \LaTeX .
- 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:

4. Define Mappings

Changed in
version 0.3

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

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.

Changed in
version 0.3

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

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.

Changed in
version 0.3

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

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.

Introduced in
version 1.0

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

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

Introduced in
version 1.0

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

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

Introduced in
version 1.0

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

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 upppercase version for the corresponding greek letter at the current position. This will become clearer if you look at how the default mapping is defined:

```

1 \newchemgreekmapping{default}
2 {
3   \ensuremath{\alpha} / \ensuremath{\mathrm{A}} , % 1: alpha
4   \ensuremath{\beta} / \ensuremath{\mathrm{B}} , % 2: beta
5   \ensuremath{\gamma} / \ensuremath{\Gamma} , % 3: gamma
6   \ensuremath{\delta} / \ensuremath{\Delta} , % 4: delta
7   \ensuremath{\epsilon} / \ensuremath{\mathrm{E}} , % 5: epsilon
8   \ensuremath{\zeta} / \ensuremath{\mathrm{Z}} , % 6: zeta
9   \ensuremath{\eta} / \ensuremath{\mathrm{H}} , % 7: eta
10  \ensuremath{\theta} / \ensuremath{\Theta} , % 8: theta
11  \ensuremath{\iota} / \ensuremath{\mathrm{I}} , % 9: iota
12  \ensuremath{\kappa} / \ensuremath{\mathrm{K}} , % 10: kappa
13  \ensuremath{\lambda} / \ensuremath{\Lambda} , % 11: lambda
14  \ensuremath{\mu} / \ensuremath{\mathrm{M}} , % 12: mu
15  \ensuremath{\nu} / \ensuremath{\mathrm{N}} , % 13: nu
16  \ensuremath{\xi} / \ensuremath{\Xi} , % 14: xi
17  \ensuremath{o} / \ensuremath{\mathrm{O}} , % 15: omikron

```

5. Predefined Mappings and Selection of a Mapping

```

18 \ensuremath{\pi}      / \ensuremath{\Pi} ,      % 16: pi
19 \ensuremath{\rho}      / \ensuremath{\mathrm{P}} , % 17: rho
20 \ensuremath{\sigma}     / \ensuremath{\Sigma} ,    % 18: sigma
21 \ensuremath{\tau}       / \ensuremath{\mathrm{T}} , % 19: tau
22 \ensuremath{\upsilon}   / \ensuremath{\Upsilon} ,   % 20: upsilon
23 \ensuremath{\phi}       / \ensuremath{\Phi} ,      % 21: phi
24 \ensuremath{\psi}       / \ensuremath{\Psi} ,      % 22: psi
25 \ensuremath{\chi}       / \ensuremath{\mathrm{X}} , % 23: chi
26 \ensuremath{\omega}     / \ensuremath{\Omega}      % 24: omega
27 }

```

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 let's 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`, `ϕ` and `Φ`

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 at begin document. If an unambiguous choice isn't possible then **CHEMGREEK** will select the 'default' mapping at begin document. If a user has selected a mapping manually in

5. Predefined Mappings and Selection of a Mapping

mapping	package
default	—
var-default	—
textgreek	textgreek [Mic11]
upgreek	upgreek [Scho3]
newtx	newtxmath [Sha13]
kpfonts	kpfonts [Cai10]
pxgreek	pxgreek [Bur11]
mathdesign	mathdesign [Pic13]
fourier	fourier [Bov05]
textalpha	textalpha [Mil13]
fontspec	fontspec [RH13]

TABLE 1: Predefined mappings.

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 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>}`

Changed in
version 1.0

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.*

```

1 % requires the 'newtxmath' package to be loaded:
2 \chemphi\ and \chemPhi, $\phi$ and $\Phi$\par
3 \selectchemgreekmapping{newtx}
4 \chemphi\ and \chemPhi, $\upphi$ and $\upPhi$

```

ϕ and Φ , ϕ and Φ
 ϕ and Φ , ϕ and Φ

6. Changing a Specific Symbol in an Existing Mapping

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.

```
1 \documentclass[margin=3pt]{standalone}
2 \usepackage{fontspec}
3 \setmainfont{Linux Libertine 0}% need a font that has the glyphs!
4 \usepackage{chemgreek}
5 \selectchemgreekmapping{fontspec}
6 \begin{document}
7 \printchemgreekalphabet
8 \end{document}
```

α β γ δ ϵ ζ η θ ι κ λ μ ν ξ \omicron π ρ σ τ υ ϕ ψ χ ω Ω

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 lowercase entry `<entry name>` in the mapping `<mapping name>`.

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

```
1 \chemalpha
2 \changechemgreeksymbol{default}{lower}{alpha}{xxx}%
3 \selectchemgreekmapping{default}
4 \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>}`

This will typeset a table (using a simple tabular environment) with all 48 characters like the one shown in table 2.

Introduced in
version 0.3

8. Additional Macros

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	\omicron	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.	psi	ψ	Ψ
23.	chi	χ	X
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: $\alpha A \beta B \gamma \Gamma \delta \Delta \epsilon E \zeta Z \eta H \theta \Theta \iota I \kappa K \lambda \Lambda \mu M \nu N \xi \Xi \omicron O \pi \Pi \rho R \sigma \Sigma \tau T \upsilon \Upsilon \phi \Phi \psi \Psi \chi X \omega \Omega$.

`\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’

$\alpha A \beta B \gamma \Gamma \delta \Delta \epsilon E \zeta Z \eta H \theta \Theta \iota I \kappa K \lambda \Lambda \mu M \nu N \xi \Xi o O \pi \Pi \rho P \sigma \Sigma \tau T \upsilon \Upsilon \phi \Phi \psi \Psi \chi X \omega \Omega$

A.2. Mapping ‘var-default’

$\alpha A \beta B \gamma \Gamma \delta \Delta \varepsilon E \zeta Z \eta H \theta \Theta \iota I \kappa K \lambda \Lambda \mu M \nu N \xi \Xi o O \pi \Pi \rho P \sigma \Sigma \tau T \upsilon \Upsilon \phi \Phi \psi \Psi \chi X \omega \Omega$

A.3. Mapping ‘textgreek’

$\alpha A \beta B \gamma \Gamma \delta \Delta \epsilon E \zeta Z \eta H \vartheta \Theta \iota I \chi K \lambda \Lambda \mu M \nu N \xi \Xi o O \pi \Pi \rho P \sigma \Sigma \tau T \upsilon \Upsilon \phi \Phi \psi \Psi \chi X \omega \Omega$

A.4. Mapping ‘upgreek’

$\alpha A \beta B \gamma \Gamma \delta \Delta \epsilon E \zeta Z \eta H \theta \Theta \iota I \kappa K \lambda \Lambda \mu M \nu N \xi \Xi o O \pi \Pi \rho R \sigma \Sigma \tau T \upsilon \Upsilon \phi \Phi \psi \Psi \chi X \omega \Omega$

A.5. Mapping ‘newtx’

$\alpha A \beta B \gamma \Gamma \delta \Delta \epsilon E \zeta Z \eta H \theta \Theta \iota I \kappa K \lambda \Lambda \mu M \nu N \xi \Xi o O \pi \Pi \rho R \sigma \Sigma \tau T \upsilon \Upsilon \phi \Phi \psi \Psi \chi X \omega \Omega$

A.6. Mapping ‘kpfonts’

$\alpha A \beta B \gamma \Gamma \delta \Delta \epsilon E \zeta Z \eta H \theta \Theta \iota I \kappa K \lambda \Lambda \mu M \nu N \xi \Xi o O \pi \Pi \rho R \sigma \Sigma \tau T \upsilon \Upsilon \phi \Phi \psi \Psi \chi X \omega \Omega$

A.7. Mapping ‘pxgreeks’

$\alpha A \beta B \gamma \Gamma \delta \Delta \epsilon E \zeta Z \eta H \theta \Theta \iota I \kappa K \lambda \Lambda \mu M \nu N \xi \Xi o O \pi \Pi \rho R \sigma \Sigma \tau T \upsilon \Upsilon \phi \Phi \psi \Psi \chi X \omega \Omega$

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

$\alpha A \beta B \gamma \Gamma \delta \Delta \epsilon E \zeta Z \eta H \theta \Theta \iota I \kappa K \lambda \Lambda \mu M \nu N \xi \Xi o O \pi \Pi \rho R \sigma \Sigma \tau T \upsilon \Upsilon \phi \Phi \psi \Psi \chi X \omega \Omega$

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

$\alpha A \beta B \gamma \Gamma \delta \Delta \epsilon E \zeta Z \eta H \theta \Theta \iota I \kappa K \lambda \Lambda \mu M \nu N \xi \Xi o O \pi \Pi \rho R \sigma \Sigma \tau T \upsilon \Upsilon \phi \Phi \psi \Psi \chi X \omega \Omega$

A.10. Mapping ‘fourier’

$\alpha A \beta B \gamma \Gamma \delta \Delta \epsilon E \zeta Z \eta H \theta \Theta \iota I \kappa K \lambda \Lambda \mu M \nu N \xi \Xi o O \pi \Pi \rho R \sigma \Sigma \tau T \upsilon \Upsilon \phi \Phi \psi \Psi \chi X \omega \Omega$

A.11. Mapping ‘textalpha’

α β γ δ ϵ ζ η θ ι κ λ μ ν ξ \omicron π ρ σ τ υ ϕ ψ χ ω

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

α β γ δ ϵ ζ η θ ι κ λ μ ν ξ \omicron π ρ σ τ υ ϕ ψ χ ω

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