

THE CHEMMACROS BUNDLE

v0.2a 2013/11/20

packages **CHEMMACROS** (v4.2c), **CHEMFORMULA** (v4.2a), **GHSYSTEM** (v4.0) and
CHEMGREEK (v0.2a)

documentation for the **CHEMGREEK** package

Clemens NIEDERBERGER

<https://bitbucket.org/cgnieder/chemmacros/>

contact@mychemistry.eu

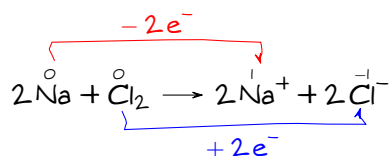


Table of Contents

1	Introduction	1	5	Changing a Specific Symbol in an Existing Mapping	4
2	Licence and Requirements	2	6	Inspecting a Mapping	5
3	Define Mappings	2		References	5
4	Predefined Mappings and Selection of a Mapping	3	Index		7

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 **CHEMMACROS** and its IUPAC naming commands.

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: `expl3`¹ [The13a] and `xparse`² [The13b].

3 Define Mappings

CHEMGREEK’s main commands are:

`\newchemgreekmapping{<name>}{<mapping list>}`

Add a new mapping to **CHEMGREEK**. Issue an error if it already exists.

`\renewchemgreekmapping{<name>}{<mapping list>}`

Renew a **CHEMGREEK** mapping. Issue an error if it doesn’t exist yet.

`\declarechemgreekmapping{<name>}{<mapping list>}`

Declare a new mapping to **CHEMGREEK**. If the mapping already exists it will be overwritten.

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:

```

1 \newchemgreekmapping{default}
2 {
3   \ensuremath{\alpha} / \ensuremath{\mathrm{A}} , % 1: alpha
4   \ensuremath{\beta} / \ensuremath{\mathrm{B}} , % 2: beta
5   \ensuremath{\gamma} / \ensuremath{\mathrm{Gamma}} , % 3: gamma
6   \ensuremath{\delta} / \ensuremath{\mathrm{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{\mathrm{Theta}} , % 8: theta
11  \ensuremath{\iota} / \ensuremath{\mathrm{I}} , % 9: iota
12  \ensuremath{\kappa} / \ensuremath{\mathrm{K}} , % 10: kappa

```

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/>

4 Predefined Mappings and Selection of a Mapping

```

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
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 `\ChemAlph`/`\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. The `CHEMMACROS` package for example provides a package option that selects one of the available mappings.

Default mapping: `\Chemphi` and `\ChemPhi`, `ϕ` and `Φ`

Default mapping: ϕ and Φ , ϕ and Φ

4 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.

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

`\activatechemgreekmapping*[\langle options \rangle]{\langle name \rangle}`

This command selects and activates the mapping `\langle name \rangle`. If the star variant is used also the package `\langle name \rangle` is loaded with options `\langle options \rangle`. This obviously only makes sense if the package name is the same as the mapping name. The command can only be used in the document preamble.

`\selectchemgreekmapping{\langle name \rangle}`

This command selects and activates the mapping `\langle name \rangle`. A required package has to be loaded

5 Changing a Specific Symbol in an Existing Mapping

additionally the usual way via `\usepackage` or `\RequirePackage`. 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

5 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:

`\changechemgreekssymbol{<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 \changechemgreekssymbol{default}{lower}{alpha}{xxx}
2 \selectchemgreekmapping{default}
3 \Chemalpha

```

xxx

mapping	package
default	—
var-default	—
textgreek	textgreek [Mic11]
upgreek	upgreek [Scho3]
newtx	newtxmath [Sha13]
kpfonts	kpfonts [Cai10]
mathdesign	mathdesign [Pic13]
fourier	fourier [Bovo5]

TABLE 1: Predefined mappings.

6 Inspecting a Mapping

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

```
\showchemgreekmapping{<mapping>}
```

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	\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 `\showchemgreekmapping` command.

References

- [Bov05] Michel Bovani. fourier. version 1.3, Jan. 30, 2005.
URL: <http://mirror.ctan.org/fonts/fourier-gut/>.
- [Cai10] Christophe Caignaert. kpfonts. version 3.31, Aug. 20, 2010.
URL: <http://mirror.ctan.org/fonts/kpfonts>.

References

- [Mic11] Leonard Michlmayr. textgreek. version 0.7, Oct. 9, 2011.
URL: <http://mirror.ctan.org/macros/latex/contrib/textgreek/>.
- [Pic13] Paul Pichaureau. mathdesign. version 2.31, Aug. 29, 2013.
URL: <http://mirror.ctan.org/fonts/mathdesign/>.
- [Scho3] Walter Schmidt. upgreek. version 2.0, Feb. 12, 2003.
URL: <http://mirror.ctan.org/macros/latex/contrib/was/>.
- [Sha13] Michael Sharpe. newtx. version 1.151, Oct. 17, 2013.
URL: <http://mirror.ctan.org/fonts/newtx/>.
- [The13a] The L^AT_EX3 Project Team. l3kernel. version SVN 4582, July 28, 2013.
URL: <http://mirror.ctan.org/macros/latex/contrib/l3kernel/>.
- [The13b] The L^AT_EX3 Project Team. l3packages. version SVN 4582, July 28, 2013.
URL: <http://mirror.ctan.org/macros/latex/contrib/l3packages/>.

Index

A	
<code>\activatechemgreekmapping</code>	3
B	
Bovani, Michel	4
C	
Caignaert, Christophe	4
<code>\changechemgreekssymbol</code>	4
<code>\ChemAlpha</code>	3
<code>\Chemalpha</code>	3 f.
<code>\ChemPhi</code>	3 f.
<code>\Chemphi</code>	3 f.
CTAN	2
D	
<code>\declarechemgreekmapping</code>	2
<code>\Delta</code>	2
E	
expl3 (package)	2
F	
fourier (package)	4
K	
kpfonts (package)	1, 4
L	
l3kernel (bundle)	2
l3packages (bundle)	2
LPPL	2
M	
mathdesign (package)	4
Michlmayr, Leonard	4
N	
<code>\newchemgreekmapping</code>	2
newtx (package)	1, 4
newtxmath (package)	4
Niederberger, Clemens	1
P	
Pichaureau, Paul	4
R	
<code>\renewchemgreekmapping</code>	2
S	
Schmidt, Walter	4
<code>\selectchemgreekmapping</code>	3 f.
Sharpe, Michael	4
<code>\showchemgreekmapping</code>	5
T	
textgreek (package)	1, 4
The L ^A T _E X ₃ Project Team	2
U	
upgreek (package)	1, 4
X	
xparse (package)	2