THE CHEMMACROS BUNDLE

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packages CHEMMACROS (v4.5a), CHEMFORMULA (v4.7), GHSYSTEM (v4.5b) and CHEMGREEK (v0.4)

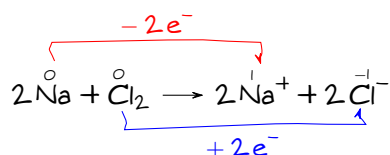## documentation for the CHEMGREEK package

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1 Introduction

The 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 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-ᴅ-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 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] [The13a] and xparse[2] [The13b].

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.

- The mapping "fourier" has been added. In order to use it you need the fourier package [Bov05] 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 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`.

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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/`

3.3 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 LuaLATEX or XƎLATEX.

- New command \printchemgreekalphabet.

4 Define Mappings

CHEMGREEK's main commands are:

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

Changed in version 0.3
Add a new mapping to CHEMGREEK. Issue an error if it 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. Issue an error if it 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.

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

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

Default mapping: ϕ and Φ, ϕ and Φ

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. Ths 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.

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

`\activatechemgreekmapping*{⟨name⟩}`

Changed in version 0.3

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. The command can only be used in the document preamble.

`\selectchemgreekmapping{⟨name⟩}`

Changed in version 0.3

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. The command can be used throughout the document.

mapping	package
default	—
var-default	—
textgreek	textgreek [Mic11]
upgreek	upgreek [Sch03]
newtx	newtxmath [Sha13]
kpfonts	kpfonts [Cai10]
mathdesign	mathdesign [Pic13]
fourier	fourier [Bov05]
textalpha	textalpha [Mil13]
fontspec	fontspec [RH13]

TABLE 1: Predefined mappings.

```
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

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 O}% need a font that has the glyphs!
4 \usepackage{chemgreek}
5 \selectchemgreekmapping{fontspec}
6 \begin{document}
7 \printchemgreekalphabet
8 \end{document}
```

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

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.

\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 oO πΠ ρR σΣ τT υϒ ϕΦ ψΨ χX 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.

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	o	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.

References

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

[Mic11]   Leonard Michlmayr. textgreek. version 0.7, Oct. 9, 2011.
           URL: http://mirror.ctan.org/macros/latex/contrib/textgreek/.

[Mil13]   Günter Milde. greek-fontenc. version 0.11.1, Dec. 1, 2013.
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[OR12]   Heiko Oberdiek and Sebastian Rahtz. hyperref. version 6.83m, Nov. 6, 2012.
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[RH13]   Will Robertson and Khaled Hosny. fontspec. version 2.3c, May 20, 2013.
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[Sch03]   Walter Schmidt. upgreek. version 2.0, Feb. 12, 2003.
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