

ELEMENTS

v0.1 2015/06/014

properties of chemical elements

Clemens NIEDERBERGER

<https://github.com/cgnieder/elements/>

contact@mychemistry.eu

This package provides means for retrieving properties of chemical elements like atomic number, element symbol, element name, electron distribution or isotope number. Properties are defined for the elements up to the atomic number 112.

This package is a spin-off of the package bohr by the same author.

Table of Contents

1	Licence and Requirements	1	5	Electron Configuration	3
2	Element Names	1	6	Isotope Lists	4
3	Element Symbols	2		References	4
4	Atomic Numbers	2		Index	4

1 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.”

ELEMENTS loads the etoolbox package [LW15].

2 Element Names

`\elementname{⟨atomic number⟩|⟨element symbol⟩}`

Prints the element name of a given element as defined with `\setatomname`.

`\setatomname[⟨alt. name⟩]{⟨atomic number⟩}{⟨element name⟩}`

Define or redefine the name of an element. If `⟨element name⟩` contains non-ascii symbols

3 Element Symbols

the optional argument $\langle alt. name \rangle$ must be given. In this case $\langle alt. name \rangle$ must be used in **ELEMENTS**' other macros where an element's name can be given as argument.

`\DeclareAtomName` $\langle alt. name \rangle$ $\{\langle atomic number \rangle\}$ $\{\langle element name \rangle\}$

This is the same as `\setatomname` but used before begin document or in packages/classes.

`\saveelementname` $\langle cs \rangle$ $\{\langle atomic number \rangle$ $\mid \langle element symbol \rangle$ $\mid \langle element name \rangle\}$

Saves the name of the given element as replacement text for the macro $\langle cs \rangle$.

1	<code>\elementname{Cu}</code>	<code>\par</code>	Copper
2	<code>\elementname{11}</code>	<code>\par</code>	Sodium
3	<code>\saveelementname\foo{28}</code>		macro:->Nickel
4	<code>\ttfamily\meaning\foo</code>		

3 Element Symbols

`\elementsymbol` $\{\langle atomic number \rangle$ $\mid \langle element name \rangle\}$

Prints the element symbol of a given element as defined with `\setatomsymbol`.

`\setatomsymbol` $\{\langle atomic number \rangle\}$ $\{\langle element symbol \rangle\}$

Define or redefine the symbol of an element.

`\DeclareAtomSymbol` $\{\langle atomic number \rangle\}$ $\{\langle element symbol \rangle\}$

This is the same as `\setatomsymbol` but used before begin document or in packages/classes.

`\saveelementsymbols` $\langle cs \rangle$ $\{\langle atomic number \rangle$ $\mid \langle element symbol \rangle$ $\mid \langle element name \rangle\}$

Saves the symbol of the given element as replacement text for the macro $\langle cs \rangle$.

1	<code>\elementsymbol{13}</code>	<code>\par</code>	Al
2	<code>\elementsymbol{Sulfur}</code>	<code>\par</code>	S
3	<code>\saveelementsymbols\foo{83}</code>		macro:->Bi
4	<code>\ttfamily\meaning\foo</code>		

4 Atomic Numbers

`\atomicnumber` $\{\langle element symbol \rangle$ $\mid \langle element name \rangle\}$

Prints the atomic number of a given element.

`\Z` $\{\langle element symbol \rangle$ $\mid \langle element name \rangle\}$

An alias of `\atomicnumber` but only defined at begin document and only if it isn't defined by any other package.

`\saveatomicnumber{⟨cs⟩}{⟨atomic number⟩|⟨element symbol⟩|⟨element name⟩}`

Saves the atomic number of the given element as replacement text for the macro `⟨cs⟩`.

<pre>1 \atomicnumber{U} \par 2 \atomicnumber{Chlorine} \par 3 \saveatomicnumber\foo{Kr} 4 \ttfamily\meaning\foo</pre>	<pre>92 17 macro:->36</pre>
---	--------------------------------

5 Electron Configuration

`\elconf{⟨atomic number⟩|⟨element symbol⟩|⟨element name⟩}`

Typesets the electron configuration of the given element.

`\writeelconf{⟨electron distribution⟩}`

Typesets the electron distribution `⟨electron distribution⟩`. The input is the same as described below for `\setelectrondistribution`.

`\setelectrondistribution{⟨atomic number⟩}{⟨electron distribution⟩}`

This set the electron distribution associated with the atom number `⟨atomic number⟩`. `⟨electron distribution⟩` is a comma-separated list of the number of electrons placed on each shell from inner to outer shell. For example `\setelectrondistribution{3}{2,0,1}` would be an excited Lithium. The number of electrons with the same principal quantum number but a different angular quantum number are separated with a + ordered by the angular quantum number, *i. e.*, first *s*, then *p*, then *d*, and then *f*. Copper's distribution would be declared like this:

`\setelectrondistribution{29}{2,2+6,2+6+10,1}`.

A declaration with `\setelectrondistribution{29}{2,8,18,1}` would work but then `\elconf{29}` would give the wrong results.

`\DeclareElectronDistribution`

This is the same as `\setelectrondistribution` but used before begin document or in packages/classes.

<pre>1 \writeelconf{2,2+6,2+6+7} \par 2 \elconf{Cl}</pre>	<pre>1s²2s²2p⁶3s²3p⁶3d⁷ 1s²2s²2p⁶3s²3p⁵</pre>
---	--

There is currently *no way* to get the electron configuration in the shortened way (*e. g.*: `[Ar]3d104s1`).

6 Isotope Lists

`\setatomisotopes{⟨atomic number⟩}{⟨isotope list⟩}`

Defines or redefines the isotope list for a given element. *⟨isotope list⟩* should be a comma separated list of integers. One of the integers may be preceded with a `!` to mark the main isotope for the given element: `\setatomisotopes{6}{10,11,!12,13,14,15,16}`

`\DeclareAtomIsotopes{⟨atomic number⟩}{⟨isotope list⟩}`

This is the same as `\setatomisotopes` but used before begin document or in packages/classes.

`\saveelementisotopes{⟨cs⟩}{⟨atomic number⟩|⟨element symbol⟩|⟨element name⟩}`

Saves the isotope list of the given element as replacement text for the macro *⟨cs⟩*.

`\savemainelementisotope{⟨cs⟩}{⟨atomic number⟩|⟨element symbol⟩|⟨element name⟩}`

Saves the main isotope of the given element as replacement text for the macro *⟨cs⟩*. If the isotope list of the element contains no main isotope *⟨cs⟩* will be equivalent to `\@empty`.

```

1 \ttfamily
2 \saveelementisotopes\foo{C}           macro: ->10,11,!12,13,14,15,16
3 \meaning\foo                          macro: ->12
4 \savemainelementisotope\foo{C}
5 \meaning\foo

```

References

[LW15] Philipp LEHMAN and Joseph WRIGHT. etoolbox. version 2.2, Apr. 4, 2015.
URL: <http://mirror.ctan.org/macros/latex/contrib/etoolbox/>.

Index

A	E	<code>\saveelementname</code> 2
<code>\atomicnumber</code> 2 f.	<code>\elconf</code> 3	<code>\saveelementsymbols</code> 2
	<code>\elementname</code> 1 f.	<code>\setatomname</code> 1 f.
	<code>\elementsymbols</code> 2	<code>\setatomsymbols</code> 2
B	etoolbox (package) 1	<code>\setelectrondistribution</code> 3
bohr (package) 1		
	L	W
D	LEHMAN, Philipp 1	WRIGHT, Joseph 1
<code>\DeclareAtomName</code> 2	LPPL 1	<code>\writeelconf</code> 3
<code>\DeclareAtomSymbol</code> 2		
<code>\DeclareElectronDistribution</code> 3	S	Z
	<code>\saveatomicnumber</code> 3	<code>\Z</code> 2