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simple atom representation according to the Bohr model

Clemens Niederberger

https://bitbucket.org/cgnieder/bohr/ contact@mychemistry.eu

English documentation

This package provides means for the creation of simple Bohr models of atoms up to the atomic number 112. Additionally commands are provided to convert atomic numbers to element symbols or element names and vice versa.

The package is inspired by a question on http://tex.stackexchange.com/: Draw Bohr atomic model with electron shells in TeX?

Contents		4		Customization	2
1	Licence and Requirements	1	5	Additional Commands	4
2	Options	1	6	Implementation	5
3	Usage	2	In	dex	15

1 Licence and Requirements

BOHR is placed under the terms of the LaTeX Project Public License, version 1.3 or later (http://www.latex-project.org/lppl.txt). It has the status "maintained."

BOHR loads and needs the packages tikz, 1 pgfopts 2 and etoolbox. 3

2 Options

Every option described in the manual can also be used as package option. Options are indicated as option and are all key/value like options. Some options can be set without value, too. Then

¹ CTAN: tikz ² CTAN: pgfopts ³ CTAN: etoolbox

the underlined value is used.

3 Usage

BOHR is used like any other LTEX 2ε package:

```
\usepackage{bohr}
```

The main command, \bohr, creates the models:

▶\bohr[<num of shells>]{<number of electrons>}{<atom name>}

This is described best by an example:

```
\bohr{3}{Li}
```

There is not much more to it. Another example using the optional argument:

```
\bohr[2]{2}{$\mathrm{Li^+}$}
```

4 Customization

BOHR provides a handful of options to customize the appearance:

▶ \setbohr{<options>}

Options are set in a key/value syntax using this command.

- ► insert-symbol = <u>true</u>|false Default: false

 If set to true BOHR will insert the atomic symbol suiting to the given electron number if *no* third argument is given.
- ▶ insert-number = true | false Default: false If set to true BOHR will use the appropriate number of electrons for the given element symbol in the third argument if *no* second argument is given. This of course only works if the third argument is one of the 112 element symbols.

▶ insert-missing = true|false
Sets both insert-symbol and insert-number.

▶ atom-style = <code>

(initially empty)

Default: false

This code will be placed immediatly before the third argument of \bohr. The last macro in it may need one argument.

▶ name-options-set = <tikz>

(initially empty)

This value is passed to the options of the \node the third argument of \bohr is placed in.

▶ name-options-add = <tikz>

(initially empty)

This value will be added to options set with name-options-set.

- ▶ nucleus-option-set = <tikz> Default: draw=black!80, fill=black!10, opacity=.25 This value is passed to the options of the \draw command that draws the circle around the name-node.
- ▶ nucleus-options-add = <tikz>

(initially empty)

This value will be added to options set with nucleus-options-set.

▶ nucleus-radius = <dim>

Default: 1em

The radius of the circle around the name-node.

▶ electron-options-set = <tikz>

Default: blue!50!black!50

This value is passed to the options of the \fill command that draws the electrons.

▶ electron-options-add = <tikz>

(initially empty)

This value will be added to options set with electron-options-set.

▶ electron-radius = <dim>

Default: 1.5pt

The radius of the circles that represent the electrons.

▶ shell-options-set = <tikz>

Default: draw=blue!75, thin

This value is passed to the options of the \draw command that draws the circles that represent the shells.

▶ shell-options-add = <tikz>

(initially empty)

This value will be added to options set with shell-options-set.

▶ shell-dist = <dim>

Default: 1em

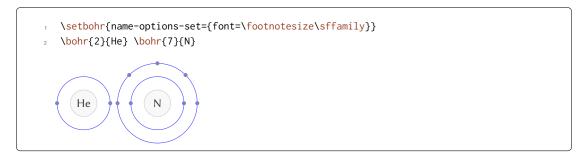
The distance between the nucleus and the first shell and between subsequent shells.

▶ german = true|false

Default: false

If set to true the German names are defined (see section 5 to understand what I mean). They are also defined if you use babel⁴ and select language german or ngerman in the preamble. The same holds for polyglossia.⁵

⁴ CTAN: babel ⁵ CTAN: polyglossia



```
1 % uses package 'chemmacros'
2 \setbohr{atom-style={\footnotesize\sffamily\ch}}
3 \bohr{0}{H+} \bohr{10}{F-}
```

5 Additional Commands

BOHR provides some additional commands that return the element symbol or the element name to a given atomic number and vice versa.

- ▶ \elementsymbol{<atomic number>|<element name>}
 - Returns the element symbol for a given atomic number or element name. $\ensuremath{\verb| elementsymbol|} \{80\}$: Hg; $\ensuremath{\verb| elementsymbol|} \{rhenium\}$: Rh.
- ▶ \elementname{<atomic number>|<element symbol>}
 Returns the element name for a given atomic number or element symbol. \elementname{80}:
 Mercury; \elementname{Rh}: Rhenium.
- ► \atomicnumber{<element name>|<element symbol>}
 Returns the atomic number for a given element name or element symbol. \atomicnumber{Hg}:
 80; \atomicnumber{rhenium} 75.
- ► \Z

If this command isn't defined by some other package it is available as an alias of \atomicnumber.

```
The elements \elementname{F}, \elementname{Cl}, \elementname{Br}, \elementname{I} and \elementname{At} are called \emph{halogens}.
```

The elements Fluorine, Chlorine, Bromine, Iodine and Astatine are called *halogens*.

6 Implementation

```
_____
  % the BOHR package
  % simple atom representation according to the Bohr model
6 % -----
  % Clemens Niederberger
  % Web: https://bitbucket.org/cgnieder/bohr/
  % E-Mail: contact@mychemistry.eu
  % -----
% Copyright 2012 Clemens Niederberger
_{13} % This work may be distributed and/or modified under the
14 % conditions of the LaTeX Project Public License, either version 1.3
  % of this license or (at your option) any later version.
  % The latest version of this license is in
  % http://www.latex-project.org/lppl.txt
  % and version 1.3 or later is part of all distributions of LaTeX
  % version 2005/12/01 or later.
% This work has the LPPL maintenance status 'maintained'.
  % The Current Maintainer of this work is Clemens Niederberger.
  % The bohr package consists of the files
  % - bohr.sty
  % - bohr_en.tex, bohr_en.pdf
  % - bohr_elements_english.def, bohr_elements_german.def
29 % - README
  % If you have any ideas, questions, suggestions or bugs to report, please
  % feel free to contact me.
  % -----
  \def\@bohr@date{2012/09/22}
  \def\@bohr@version{v0.2}
  \def\@bohr@description{simple atom representation according to the Bohr model}
  \ProvidesPackage{bohr}[\@bohr@date\space \@bohr@version\space \@bohr@description]
  \RequirePackage{tikz,etoolbox,pgfopts}
40
```

```
% message handling
   \def\@bohr@create@message#1{%
     \ifstrequal{#1}{Error}
44
       {%
45
         \lowercase{\csdef{@bohr@#1}}##1##2{%
46
           \csuse{Package#1}{bohr}{##1}{##2}}%
48
         \lowercase{\csdef{@bohr@#1}}##1{%
           \csuse{Package#1}{bohr}{##1}}%
       }}
   \@bohr@create@message{Error}
52
   \@bohr@create@message{Warning}
   \@bohr@create@message{WarningNoLine}
   \@bohr@create@message{Info}
56
57
   % the \bohr command
       optional #1: number of shells
       #2: number of electrons
       #3: atom name
61
   63
   \def\@bohr#1#2#3{%
64
     \ifblank{#2}% electron number given ?
65
66
         \ifboolexpr{ bool {bohr@insert@number} and test {\ifblank{#3}} }
67
           {%
68
             \@bohr@error{I can't insert the electron number.}
69
               {I can't insert the electron number. You haven't specified the
               element.}%
           }{%
             \ifboolexpr
                 bool {bohr@insert@number} and not
75
                 test {\lowercase{\ifcsvoid{@bohr@atom@number@#3}}}
               }
               {%
                 \lowercase{%
                   \def\@bohr@electron@current@number{\csuse{@bohr@atom@number@#3}}}%
               }{%
                 \@bohr@error{You must specify an electron number, possibly 0.}
                   {You must specify an electron number, possibly 0.}%
83
               }%
84
           }%
85
       }{% yes
         \ifnum#2<0\relax
87
           \@bohr@error{The electron number cannot be negative!}
88
             {The electron number cannot be negative!}%
```

```
\def\@bohr@electron@current@number{#2}%
          \fi
        }%
93
      \ifblank{#1}
94
        {\@bohr@get@shell@num{\@bohr@electron@current@number}}
95
          \@bohr@get@shell@num{\@bohr@electron@current@number}%
97
          \ifnum#1<\@bohr@shell@num
            \@bohr@warning{The shell number you provided (#1) is too small for the
              electron number you provided (\@bohr@electron@current@number)! I'll
              use \@bohr@shell@num\space shells.}%
101
          \else
102
            \ifnum#1>7\relax
103
              \@bohr@warning{I know only of 7 electron shells. You gave me #1 so I'll
                be using 7 instead.}
              \def\@bohr@shell@num{7}%
              \def\@bohr@shell@num{#1}%
            \fi
          \fi
110
        }%
111
      \tikzpicture[baseline=(nucleus.base)]
112
        \expandafter\node\expandafter[\@bohr@name@options]
113
          (nucleus) at (0,0) {\@bohr@insert@symbol{\@bohr@electron@current@number}{#3}}
114
        \expandafter\draw\expandafter[\@bohr@nucleus@options]
          (nucleus) circle (\@bohr@nucleus@radius);
116
        \foreach\@bohr@current@shell@num in {1,...,\@bohr@shell@num}
117
118
            \expandafter\draw\expandafter[\@bohr@shell@options]
119
              (nucleus) circle (\@bohr@nucleus@radius+\@bohr@current@shell@num*\
      @bohr@shell@dist) ;
        \@bohr@draw@electrons{\@bohr@electron@current@number}
      \endtikzpicture
123
124
    }
125
    \def\@bohr@get@shell@num#1{%
126
      \ifnum#1<3\relax
127
        \def\@bohr@shell@num{1}%
128
      \else
        \ifnum#1<11\relax
130
          \def\@bohr@shell@num{2}%
131
        \else
132
          \ifnum#1<19\relax
133
            \def\@bohr@shell@num{3}%
134
          \else
135
            \ifnum#1<37\relax
```

```
\def\@bohr@shell@num{4}%
          \else
138
            \ifnum#1<55\relax
              \def\@bohr@shell@num{5}%
            \else
141
              \ifnum#1<87\relax
142
                \def\@bohr@shell@num{6}%
              \else
                \ifnum#1<110\relax
                 \def\@bohr@shell@num{7}%
                \else
                 \def\@bohr@shell@num{112}%
148
                 \@bohr@warning{I only know atoms up to 112 (Copernicium). You
149
                   gave me #1 so I am using 112 instead.}
                \fi
              \fi
152
            \fi
          \fi
        \fi
155
      \fi
156
     \fi
157
158
   }
159
   \def\@bohr@distribute@electrons#1#2#3#4{%
160
     \pgfmathparse{#2}%
161
     \let\@bohr@last@electron\pgfmathresult
     \foreach\@bohr@electron@number in {#1,...,\@bohr@last@electron}
164
        \expandafter\fill\expandafter[\@bohr@electron@options] (nucleus)
165
          ++(\#3*\@bohr@electron@number-\#3:\@bohr@nucleus@radius+\#4*\@bohr@shell@dist)
          circle (\@bohr@electron@radius) ;
      }
168
   }
169
   \def\@bohr@draw@electrons#1{%
     \ifnum#1<1\relax\else
172
       \ifnum#1<3\relax
173
        \ensuremath{\mbox{\mbox{$0$}}}\
      \else
        \ifnum#1<11\relax
          \else
179
          \ifnum#1<19\relax
180
            181
            \@bohr@distribute@electrons{1}{#1-10}{45}{3}%
183
          \else
184
            \ifnum#1<37\relax
```

```
\@bohr@distribute@electrons{1}{2}{180}{1}%
186
               \@bohr@distribute@electrons{1}{8}{45}{2}%
               \@bohr@distribute@electrons{1}{8}{45}{3}%
               \@bohr@distribute@electrons{1}{#1-18}{20}{4}%
             \else
190
              \ifnum#1<55\relax
                \@bohr@distribute@electrons{1}{8}{45}{2}%
                \@bohr@distribute@electrons{1}{8}{45}{3}%
                \ensuremath{\mbox{\mbox{$0$}}}\
              \else
                \ifnum#1<87\relax
198
                  \@bohr@distribute@electrons{1}{2}{180}{1}%
                  \@bohr@distribute@electrons{1}{8}{45}{2}%
                  \@bohr@distribute@electrons{1}{8}{45}{3}%
                  \@bohr@distribute@electrons{1}{18}{20}{4}%
                  \@bohr@distribute@electrons{1}{18}{20}{5}%
                  \@bohr@distribute@electrons{1}{#1-54}{11.25}{6}%
                \else
205
                  \ifnum#1<113\relax
206
                    \@bohr@distribute@electrons{1}{2}{180}{1}%
                    \@bohr@distribute@electrons{1}{8}{45}{2}%
                    \@bohr@distribute@electrons{1}{8}{45}{3}%
                    \@bohr@distribute@electrons{1}{18}{20}{4}%
                    \@bohr@distribute@electrons{1}{18}{20}{5}%
                    \@bohr@distribute@electrons{1}{32}{11.25}{6}%
                    \@bohr@distribute@electrons{1}{#1-86}{11.25}{7}%
                  \fi
214
                \fi
              \fi
216
             \fi
           \fi
218
         \fi
       \fi
221
222
   }
224
   % atomic numbers and element symbols and names
   \csdef{@bohr@atom@symbol@num@\romannumeral#1}{#2}%
     \lowercase{\csdef{@bohr@atom@number@#2}}{#1}}
228
   \def\@bohr@define@atom@name#1#2{%
229
     \csdef{@bohr@atom@name@\romannumeral#1}{#2}%
     \lowercase{\csdef{@bohr@atom@name@num@#2}}{#1}}
231
   \newrobustcmd*\DeclareAtomName[2]{%
     \@bohr@define@atom@name{#1}{#2}}
```

```
\newrobustcmd*\DeclareAtomSymbol[2]{%
      \@bohr@define@atom@symbol{#1}{#2}}
236
237
    \def\@bohr@get@atom@symbol#1{%
238
      \csuse{@bohr@atom@symbol@num@\romannumeral#1}}
239
    \def\@bohr@get@atom@number#1{%
240
      \lowercase{\csuse{@bohr@atom@number@#1}}}
    \def\@bohr@get@atom@name#1{%
242
      \csuse{@bohr@atom@name@\romannumeral#1}}
243
    \def\@bohr@element@symbol#1{%
245
      \lowercase{\ifcsdef{@bohr@atom@name@num@#1}}
246
        {\lowercase{\@bohr@get@atom@symbol{\csuse{@bohr@atom@name@num@#1}}}}
247
        {\@bohr@get@atom@symbol{#1}}}
248
    \def\@bohr@atomic@number#1{%
      \lowercase{\ifcsdef{@bohr@atom@number@#1}}
251
        {\@bohr@get@atom@number{#1}}
         \{\label{lowercase} $$ \{\csuse{@bohr@atom@name@num@#1}}\} $$
253
254
    \def\@bohr@elemt@symbol#1{%
255
      \if!\ifnum9<1#1!\@bohr@get@atom@name{#1}\fi
256
257
        \lowercase{\@bohr@get@atom@name{\csuse{@bohr@atom@number@#1}}}%
258
      \fi}
    \newrobustcmd*\elementsymbol[1]{\@bohr@element@symbol{#1}}
    \newrobustcmd*\atomicnumber[1]{\@bohr@atomic@number{#1}}
262
    \newrobustcmd*\elementname[1]{\@bohr@elemt@symbol{#1}}
263
    \left\{ \left( Z_{s}^{t} \right) \right\}
265
    \DeclareAtomSymbol{1}{H}
    \DeclareAtomSymbol{2}{He}
    \DeclareAtomSymbol{3}{Li}
    \DeclareAtomSymbol{4}{Be}
    \DeclareAtomSymbol(5){B}
    \DeclareAtomSymbol{6}{C}
    \DeclareAtomSymbol{7}{N}
    \DeclareAtomSymbol{8}{0}
    \DeclareAtomSymbol{9}{F}
    \DeclareAtomSymbol{10}{Ne}
    \DeclareAtomSymbol{11}{Na}
    \DeclareAtomSymbol{12}{Mg}
    \DeclareAtomSymbol{13}{Al}
    \DeclareAtomSymbol{14}{Si}
    \DeclareAtomSymbol{15}{P}
    \DeclareAtomSymbol{16}{S}
    \DeclareAtomSymbol{17}{Cl}
    \DeclareAtomSymbol{18}{Ar}
```

- \DeclareAtomSymbol{19}{K}
- \DeclareAtomSymbol{20}{Ca} 285
 - \DeclareAtomSymbol{21}{Sc}
- \DeclareAtomSymbol{22}{Ti}
- \DeclareAtomSymbol{23}{V} 288
- \DeclareAtomSymbol{24}{Cr} 289
- \DeclareAtomSymbol{25}{Mn}
- \DeclareAtomSymbol{26}{Fe}
- \DeclareAtomSymbol{27}{Co}
- \DeclareAtomSymbol{28}{Ni}
- \DeclareAtomSymbol{29}{Cu}
- \DeclareAtomSymbol{30}{Zn} 295
- \DeclareAtomSymbol{31}{Ga} 296
- \DeclareAtomSymbol{32}{Ge} 297
- \DeclareAtomSymbol{33}{As}
- \DeclareAtomSymbol{34}{Se} 299
- \DeclareAtomSymbol{35}{Br}
- \DeclareAtomSymbol{36}{Kr}
- \DeclareAtomSymbol{37}{Rb} 302
- \DeclareAtomSymbol{38}{Sr} 303
- \DeclareAtomSymbol{39}{Y} 304
- \DeclareAtomSymbol{40}{Zr}
- \DeclareAtomSymbol{41}{Nb} 306
- \DeclareAtomSymbol{42}{Mo}
- \DeclareAtomSymbol{43}{Tc}
- $\verb|\DeclareAtomSymbol{44}{Ru}|$
- \DeclareAtomSymbol{45}{Rh}
- \DeclareAtomSymbol{46}{Pd} 311
- \DeclareAtomSymbol{47}{Ag} 312
- \DeclareAtomSymbol{48}{Cd} 313
- \DeclareAtomSymbol{49}{In} 314
- \DeclareAtomSymbol{50}{Sn} 315
- \DeclareAtomSymbol{51}{Sb} 316
- \DeclareAtomSymbol{52}{Te}
- \DeclareAtomSymbol{53}{I} 318
- \DeclareAtomSymbol{54}{Xe} 319
- \DeclareAtomSymbol{55}{Cs}
- \DeclareAtomSymbol{56}{Ba}
- \DeclareAtomSymbol{57}{La}
- \DeclareAtomSymbol{58}{Ce}
- \DeclareAtomSymbol{59}{Pr}
- \DeclareAtomSymbol(60){Nd} 325
- \DeclareAtomSymbol{61}{Pm} 326 \DeclareAtomSymbol{62}{Sm}
- \DeclareAtomSymbol{63}{Eu}

327

- 328
- \DeclareAtomSymbol{64}{Gd} 329 \DeclareAtomSymbol{65}{Tb} 330
- \DeclareAtomSymbol{66}{Dy}
- 331 \DeclareAtomSymbol{67}{Ho}

```
\DeclareAtomSymbol{68}{Er}
333
    \DeclareAtomSymbol{69}{Tm}
334
    \DeclareAtomSymbol{70}{Yb}
335
    \DeclareAtomSymbol{71}{Lu}
336
    \DeclareAtomSymbol{72}{Hf}
337
    \DeclareAtomSymbol{73}{Ta}
338
    \DeclareAtomSymbol{74}{W}
    \DeclareAtomSymbol{75}{Rh}
340
    \DeclareAtomSymbol{76}{0s}
341
    \DeclareAtomSymbol{77}{Ir}
    \DeclareAtomSymbol{78}{Pt}
343
    \DeclareAtomSymbol{79}{Au}
344
    \DeclareAtomSymbol{80}{Hg}
345
    \DeclareAtomSymbol{81}{Tl}
346
    \DeclareAtomSymbol{82}{Pb}
    \DeclareAtomSymbol{83}{Bi}
348
    \DeclareAtomSymbol{84}{Po}
349
    \DeclareAtomSymbol{85}{At}
    \DeclareAtomSymbol{86}{Rn}
351
    \DeclareAtomSymbol{87}{Fr}
352
    \DeclareAtomSymbol{88}{Ra}
353
    \DeclareAtomSymbol{89}{Ac}
    \DeclareAtomSymbol{90}{Th}
355
    \DeclareAtomSymbol{91}{Pa}
356
    \DeclareAtomSymbol{92}{U}
    \DeclareAtomSymbol{93}{Np}
    \DeclareAtomSymbol{94}{Pu}
    \DeclareAtomSymbol{95}{Am}
360
    \DeclareAtomSymbol{96}{Cm}
361
    \DeclareAtomSymbol{97}{Bk}
    \DeclareAtomSymbol{98}{Cf}
363
    \DeclareAtomSymbol{99}{Es}
    \DeclareAtomSymbol{100}{Fm}
    \DeclareAtomSymbol{101}{Md}
    \DeclareAtomSymbol{102}{No}
    \DeclareAtomSymbol{103}{Lr}
368
    \DeclareAtomSymbol{104}{Rf}
    \DeclareAtomSymbol{105}{Db}
    \DeclareAtomSymbol{106}{Sg}
371
    \DeclareAtomSymbol{107}{Bh}
    \DeclareAtomSymbol{108}{Hs}
    \DeclareAtomSymbol{109}{Mt}
374
    \DeclareAtomSymbol{110}{Ds}
375
    \DeclareAtomSymbol{111}{Rg}
376
    \DeclareAtomSymbol{112}{Cn}
378
    % element names are defined in bohr_elements_english.def or
379
    % bohr_elements_german.def, respectively. Now we need to decide
    % which ones we want
```

```
\AfterEndPreamble{
   \ifdef\bbl@afterfi{}{\long\def\bbl@afterfi#1{\fi#1}}
   \ifboolexpr
385
       test {\iflanguage{german}} or
386
       test {\iflanguage{ngerman}}
387
388
     {\booltrue{bohr@german}}{}
   \ifbool{bohr@german}
     {\input{bohr_elements_german.def}}
     {\input{bohr_elements_english.def}}
393
394
   % options
397
   \def\@bohr@name@options{}
   \def\@bohr@write@atom#1{#1}
   \def\@bohr@nucleus@radius{1em}
   \def\@bohr@electron@options{blue!50!black!50}
   \def\@bohr@electron@radius{1.5pt}
   \def\@bohr@shell@dist{1em}
   \def\@bohr@nucleus@options{draw=black!80,fill=black!10,opacity=.25}
   \def\@bohr@shell@options{draw=blue!75,thin}
405
   \newbool{bohr@insert@symbol}
   \newbool{bohr@insert@number}
    \newbool{bohr@german}
409
410
   \def\@bohr@insert@symbol#1#2{%
      \ifbool{bohr@insert@symbol}
412
       413
       {\@bohr@write@atom{#2}}}
414
   \pgfkeys{
416
     bohr/.cd,
417
       insert-symbol/.is if
                                  = bohr@insert@symbol ,
418
                                  = bohr@insert@number ,
       insert-number/.is if
       insert-missing/.is choice,
       insert-missing/true/.code =
         \booltrue{bohr@insert@symbol}\booltrue{bohr@insert@number} ,
       insert-missing/false/.code =
         \boolfalse{bohr@insert@symbol}\boolfalse{bohr@insert@number} ,
424
       insert-missing/.default
                                  = true ,
425
       atom-style/.code
                                  = \def\@bohr@write@atom{#1} ,
                                  = \def\@bohr@name@options{#1},
       name-options-set/.code
       name-options-add/.code
428
         \expandafter\def\expandafter\@bohr@name@options\expandafter{\
     @bohr@name@options,#1} ,
```

```
nucleus-radius/.code
                                  = \def\@bohr@nucleus@radius{#1} ,
430
       nucleus-options-set/.code = \def\@bohr@nucleus@options{#1} ,
431
       nucleus-options-add/.code =
         \expandafter\def\expandafter\@bohr@nucleus@options\expandafter{\
433
     @bohr@nucleus@options,#1} ,
       electron-radius/.code
                                  = \def\@bohr@electron@radius{#1} ,
434
       electron-options-set/.code = \def\@bohr@electron@options{#1} ,
435
       electron-options-add/.code =
436
         \expandafter\def\expandafter\@bohr@electron@options\expandafter{\
437
     @bohr@electron@options,#1} ,
       shell-dist/.code
                                  = \def\@bohr@shell@dist{#1} ,
       shell-options-set/.code
                                  = \def\@bohr@shell@options{#1} ,
439
       shell-options-add/.code
440
         441
     @bohr@shell@options,#1} ,
                                  = bohr@german ,
       german/.is if
442
       ngerman/.is if
                                  = bohr@german
443
   }
445
   \newrobustcmd\setbohr[1]{\pgfqkeys{/bohr}{#1}}
446
447
   \ProcessPgfOptions*
   \endinput
449
450
   % HISTORY
451
   2012/09/21 v0.1a - first version on bitbucket
   2012/09/22 v0.2 - added compatibility up to atomic number 112
453
                     - added the commands \elementname and \elementsymbol with
454
                      language support German and English
                    - improved error checking
```

Index

A	N	
atom-style3	$\verb name-options-add3 $	
\atomicnumber4	name-options-set3	
	nucleus-option-set3	
В	nucleus-options-add3	
babel	nucleus-options-set3	
\bohr 2 f.	nucleus-radius3	
C	О	
Customization 2 ff.	option1	
	Options 1 f.	
E	n.	
electron-options-add3	P	
electron-options-set3	pgfopts 1	
electron-radius 3	polyglossia	
\elementname 4	S	
\elementsymbol4	\setbohr2	
etoolbox1	shell-dist3	
	shell-options-add3	
G	shell-options-set3	
${\tt german3}$,	
I	T	
insert-missing3	tikz1	
insert-number	IJ	
insert-symbol	· ·	
Triber & Symbol	Usage2	
L	Z	
License	\ <mark>Z</mark>	