BOHR

0.2 2012/09/22

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

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 LaTeX 2_ε package:

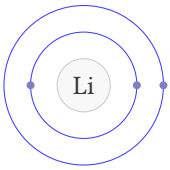
```
\usepackage{bohr}
```

The main command, \bohr, creates the models:

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

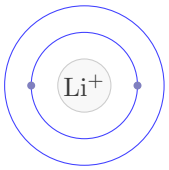
This is described best by an example:

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

▸ `insert-symbol = true|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.

▸ `atom-style = <code>` (initially empty)
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.

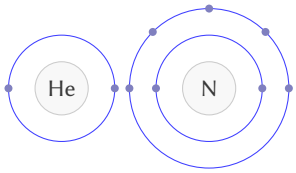
▸ `shell-options-add = <tikz>` (initially empty)
This value will be added to options set with `shell-options-set`.

▸ `shell-dist = <dim>` Default: `1em`
The distance between the nucleus and the first shell and between subsequent shells.

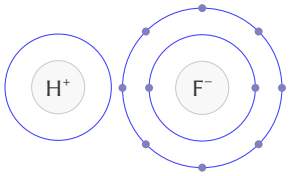
▸ `german = true|false` Default: `false`
If set to `true` the German names are defined (see section 5 to understand what I mean). They are also defined if you use babel[4] and select language `german` or `ngerman` in the preamble. The same holds for polyglossia.[5]

```
\setbohr{name-options-set={font=\footnotesize\sffamily}}
\bohr{2}{He} \bohr{7}{N}
```

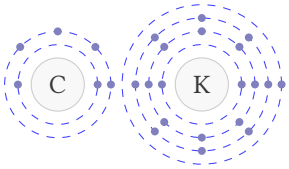
[4] CTAN: babel [5] CTAN: polyglossia




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




```
\setbohr{
  shell-options-add = dashed,
  shell-dist        = .5em,
  insert-symbol
}
\bohr{6}{} \bohr{19}{}
```



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. `\elementsymbol{80}`: Hg; `\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`. `\Z{Hg}`: *(Z)*Hg.

```
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
%
% ------------------------------------------------------------------------------

% Clemens Niederberger
% Web:    https://bitbucket.org/cgnieder/bohr/
% E-Mail: contact@mychemistry.eu
% ------------------------------------------------------------------------------

% Copyright 2011-2012 Clemens Niederberger
%
% This work may be distributed and/or modified under the
% 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
%  - 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{0.2}
\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}

% ------------------------------------------------------------------------

% message handling
\def\@bohr@create@message#1{%
  \ifstrequal{#1}{Error}
    {%
      \lowercase{\csdef{@bohr@#1}}##1##2{%
        \csuse{Package#1}{bohr}{##1}{##2}}%
    }{%
      \lowercase{\csdef{@bohr@#1}}##1{%
        \csuse{Package#1}{bohr}{##1}}%
    }}
\@bohr@create@message{Error}
\@bohr@create@message{Warning}
\@bohr@create@message{WarningNoLine}
\@bohr@create@message{Info}

% ------------------------------------------------------------------------

% the \bohr command
%   optional #1: number of shells
%   #2: number of electrons
%   #3: atom name
\newrobustcmd*\bohr[3][]{\@bohr{#1}{#2}{#3}}

\def\@bohr#1#2#3{%
  \ifblank{#2}
    {%
      \@bohr@error{You must specify an electron number, possibly 0.}
        {You must specify an electron number, possibly 0.}%
    }{%
      \ifnum#2<0\relax
        \@bohr@error{The electron number cannot be negative!}
          {The electron number cannot be negative!}%
      \fi
    }%
  \ifblank{#1}
    {\@bohr@get@shell@num{#2}}
    {
      \@bohr@get@shell@num{#2}%
      \ifnum#1<\@bohr@shell@num
```

```
        \@bohr@warning{The shell number you provided (#1) is too small for
    the
          electron number you provided (#2)! I'll use \@bohr@shell@num\
    space shells.}%
      \else
        \ifnum#1>7\relax
          \@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}%
        \else
          \def\@bohr@shell@num{#1}%
        \fi
      \fi
    }%
  \tikzpicture[baseline=(nucleus.base)]
    \expandafter\node\expandafter[\@bohr@name@options]
      (nucleus) at (0,0) {\@bohr@insert@symbol{#2}{#3}} ;
    \expandafter\draw\expandafter[\@bohr@nucleus@options]
      (nucleus) circle (\@bohr@nucleus@radius) ;
    \foreach\@bohr@current@shell@num in {1,...,\@bohr@shell@num}
      {
        \expandafter\draw\expandafter[\@bohr@shell@options]
          (nucleus) circle (\@bohr@nucleus@radius+\@bohr@current@shell@num*\
    @bohr@shell@dist) ;
      }
    \@bohr@draw@electrons{#2}
  \endtikzpicture
}

\def\@bohr@get@shell@num#1{%
  \ifnum#1<3\relax
    \def\@bohr@shell@num{1}%
  \else
    \ifnum#1<11\relax
      \def\@bohr@shell@num{2}%
    \else
      \ifnum#1<19\relax
        \def\@bohr@shell@num{3}%
      \else
        \ifnum#1<37\relax
          \def\@bohr@shell@num{4}%
        \else
          \ifnum#1<55\relax
            \def\@bohr@shell@num{5}%
          \else
            \ifnum#1<87\relax
              \def\@bohr@shell@num{6}%
            \else
```

```
                \ifnum#1<110\relax
                  \def\@bohr@shell@num{7}%
                \else
                  \def\@bohr@shell@num{112}%
                  \@bohr@warning{I only know atoms up to 112 (Copernicium).
  You
                    gave me #1 so I am using 112 instead.}
                \fi
              \fi
            \fi
          \fi
        \fi
      \fi
    \fi
  \fi
}

\def\@bohr@distribute@electrons#1#2#3#4{%
  \pgfmathparse{#2}%
  \let\@bohr@last@electron\pgfmathresult
  \foreach\@bohr@electron@number in {#1,...,\@bohr@last@electron}
    {
      \expandafter\fill\expandafter[\@bohr@electron@options] (nucleus)
        ++(#3*\@bohr@electron@number-#3:\@bohr@nucleus@radius+#4*\
  @bohr@shell@dist)
        circle (\@bohr@electron@radius) ;
    }
}

\def\@bohr@draw@electrons#1{%
  \ifnum#1<1\relax\else
    \ifnum#1<3\relax
      \@bohr@distribute@electrons{1}{#1}{180}{1}%
    \else
      \ifnum#1<11\relax
        \@bohr@distribute@electrons{1}{2}{180}{1}%
        \@bohr@distribute@electrons{1}{#1-2}{45}{2}%
      \else
        \ifnum#1<19\relax
          \@bohr@distribute@electrons{1}{2}{180}{1}%
          \@bohr@distribute@electrons{1}{8}{45}{2}%
          \@bohr@distribute@electrons{1}{#1-10}{45}{3}%
        \else
          \ifnum#1<37\relax
            \@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}{#1-18}{20}{4}%
          \else
            \ifnum#1<55\relax
```

```
                \@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}{#1-36}{20}{5}%
              \else
                \ifnum#1<87\relax
                  \@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
                  \ifnum#1<113\relax
                    \@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
                \fi
              \fi
            \fi
          \fi
        \fi
      \fi
    \fi
  \fi
}

% ---------------------------------------------------------------------------

% atomic numbers and element symbols and names
\def\@bohr@define@atom@symbol#1#2{%
  \csdef{@bohr@atom@symbol@num@\romannumeral#1}{#2}%
  \lowercase{\csdef{@bohr@atom@number@#2}}{#1}}
\def\@bohr@define@atom@name#1#2{%
  \csdef{@bohr@atom@name@\romannumeral#1}{#2}%
  \lowercase{\csdef{@bohr@atom@name@num@#2}}{#1}}

\newrobustcmd*\DeclareAtomName[2]{%
  \@bohr@define@atom@name{#1}{#2}}
\newrobustcmd*\DeclareAtomSymbol[2]{%
  \@bohr@define@atom@symbol{#1}{#2}}

\def\@bohr@get@atom@symbol#1{%
  \csuse{@bohr@atom@symbol@num@\romannumeral#1}}
```

```
\def\@bohr@get@atom@number#1{%
  \lowercase{\csuse{@bohr@atom@number@#1}}}
\def\@bohr@get@atom@name#1{%
  \csuse{@bohr@atom@name@\romannumeral#1}}

\def\@bohr@element@symbol#1{%
  \lowercase{\ifcsdef{@bohr@atom@name@num@#1}}
    {\lowercase{\@bohr@get@atom@symbol{\csuse{@bohr@atom@name@num@#1}}}}
    {\@bohr@get@atom@symbol{#1}}}

\def\@bohr@atomic@number#1{%
  \lowercase{\ifcsdef{@bohr@atom@number@#1}}
    {\@bohr@get@atom@number{#1}}
    {\lowercase{\csuse{@bohr@atom@name@num@#1}}}}
\ifdef\Z{}{\let\Z\atomicnumber}

\def\@bohr@elemt@symbol#1{%
  \if!\ifnum9<1#1!\@bohr@get@atom@name{#1}\fi
  \else
    \lowercase{\@bohr@get@atom@name{\csuse{@bohr@atom@number@#1}}}%
  \fi}

\newrobustcmd*\elementsymbol[1]{\@bohr@element@symbol{#1}}
\newrobustcmd*\atomicnumber[1]{\@bohr@atomic@number{#1}}
\newrobustcmd*\elementname[1]{\@bohr@elemt@symbol{#1}}

\DeclareAtomSymbol{1}{H}
\DeclareAtomSymbol{2}{He}
\DeclareAtomSymbol{3}{Li}
\DeclareAtomSymbol{4}{Be}
\DeclareAtomSymbol{5}{B}
\DeclareAtomSymbol{6}{C}
\DeclareAtomSymbol{7}{N}
\DeclareAtomSymbol{8}{O}
\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}
\DeclareAtomSymbol{21}{Sc}
\DeclareAtomSymbol{22}{Ti}
\DeclareAtomSymbol{23}{V}
```

```
\DeclareAtomSymbol{24}{Cr}
\DeclareAtomSymbol{25}{Mn}
\DeclareAtomSymbol{26}{Fe}
\DeclareAtomSymbol{27}{Co}
\DeclareAtomSymbol{28}{Ni}
\DeclareAtomSymbol{29}{Cu}
\DeclareAtomSymbol{30}{Zn}
\DeclareAtomSymbol{31}{Ga}
\DeclareAtomSymbol{32}{Ge}
\DeclareAtomSymbol{33}{As}
\DeclareAtomSymbol{34}{Se}
\DeclareAtomSymbol{35}{Br}
\DeclareAtomSymbol{36}{Kr}
\DeclareAtomSymbol{37}{Rb}
\DeclareAtomSymbol{38}{Sr}
\DeclareAtomSymbol{39}{Y}
\DeclareAtomSymbol{40}{Zr}
\DeclareAtomSymbol{41}{Nb}
\DeclareAtomSymbol{42}{Mo}
\DeclareAtomSymbol{43}{Tc}
\DeclareAtomSymbol{44}{Ru}
\DeclareAtomSymbol{45}{Rh}
\DeclareAtomSymbol{46}{Pd}
\DeclareAtomSymbol{47}{Ag}
\DeclareAtomSymbol{48}{Cd}
\DeclareAtomSymbol{49}{In}
\DeclareAtomSymbol{50}{Sn}
\DeclareAtomSymbol{51}{Sb}
\DeclareAtomSymbol{52}{Te}
\DeclareAtomSymbol{53}{I}
\DeclareAtomSymbol{54}{Xe}
\DeclareAtomSymbol{55}{Cs}
\DeclareAtomSymbol{56}{Ba}
\DeclareAtomSymbol{57}{La}
\DeclareAtomSymbol{58}{Ce}
\DeclareAtomSymbol{59}{Pr}
\DeclareAtomSymbol{60}{Nd}
\DeclareAtomSymbol{61}{Pm}
\DeclareAtomSymbol{62}{Sm}
\DeclareAtomSymbol{63}{Eu}
\DeclareAtomSymbol{64}{Gd}
\DeclareAtomSymbol{65}{Tb}
\DeclareAtomSymbol{66}{Dy}
\DeclareAtomSymbol{67}{Ho}
\DeclareAtomSymbol{68}{Er}
\DeclareAtomSymbol{69}{Tm}
\DeclareAtomSymbol{70}{Yb}
\DeclareAtomSymbol{71}{Lu}
\DeclareAtomSymbol{72}{Hf}
```

```
\DeclareAtomSymbol{73}{Ta}
\DeclareAtomSymbol{74}{W}
\DeclareAtomSymbol{75}{Rh}
\DeclareAtomSymbol{76}{Os}
\DeclareAtomSymbol{77}{Ir}
\DeclareAtomSymbol{78}{Pt}
\DeclareAtomSymbol{79}{Au}
\DeclareAtomSymbol{80}{Hg}
\DeclareAtomSymbol{81}{Tl}
\DeclareAtomSymbol{82}{Pb}
\DeclareAtomSymbol{83}{Bi}
\DeclareAtomSymbol{84}{Po}
\DeclareAtomSymbol{85}{At}
\DeclareAtomSymbol{86}{Rn}
\DeclareAtomSymbol{87}{Fr}
\DeclareAtomSymbol{88}{Ra}
\DeclareAtomSymbol{89}{Ac}
\DeclareAtomSymbol{90}{Th}
\DeclareAtomSymbol{91}{Pa}
\DeclareAtomSymbol{92}{U}
\DeclareAtomSymbol{93}{Np}
\DeclareAtomSymbol{94}{Pu}
\DeclareAtomSymbol{95}{Am}
\DeclareAtomSymbol{96}{Cm}
\DeclareAtomSymbol{97}{Bk}
\DeclareAtomSymbol{98}{Cf}
\DeclareAtomSymbol{99}{Es}
\DeclareAtomSymbol{100}{Fm}
\DeclareAtomSymbol{101}{Md}
\DeclareAtomSymbol{102}{No}
\DeclareAtomSymbol{103}{Lr}
\DeclareAtomSymbol{104}{Rf}
\DeclareAtomSymbol{105}{Db}
\DeclareAtomSymbol{106}{Sg}
\DeclareAtomSymbol{107}{Bh}
\DeclareAtomSymbol{108}{Hs}
\DeclareAtomSymbol{109}{Mt}
\DeclareAtomSymbol{110}{Ds}
\DeclareAtomSymbol{111}{Rg}
\DeclareAtomSymbol{112}{Cn}

% element names are defined in bohr_elements_english.def or
% 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
  {
    test {\iflanguage{german}} or
```

```
    test {\iflanguage{ngerman}}
  }
  {\booltrue{bohr@german}}{}
\ifbool{bohr@german}
  {\input{bohr_elements_german.def}}
  {\input{bohr_elements_english.def}}
}


% ---------------------------------------------------------------------------

% options
\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}

\newbool{bohr@insert@symbol}
\newbool{bohr@german}

\def\@bohr@insert@symbol#1#2{%
  \ifbool{bohr@insert@symbol}
    {\ifblank{#2}{\@bohr@get@atom@symbol{#1}}{\@bohr@write@atom{#2}}}
    {\@bohr@write@atom{#2}}}

\pgfkeys{
  bohr/.cd,
    insert-symbol/.is if       = bohr@insert@symbol ,
    atom-style/.code           = \def\@bohr@write@atom{#1} ,
    name-options-set/.code     = \def\@bohr@name@options{#1} ,
    name-options-add/.code     =
      \expandafter\def\expandafter\@bohr@name@options\expandafter{\
@bohr@name@options,#1} ,
    nucleus-radius/.code       = \def\@bohr@nucleus@radius{#1} ,
    nucleus-options-set/.code  = \def\@bohr@nucleus@options{#1} ,
    nucleus-options-add/.code  =
      \expandafter\def\expandafter\@bohr@nucleus@options\expandafter{\
@bohr@nucleus@options,#1} ,
    electron-radius/.code      = \def\@bohr@electron@radius{#1} ,
    electron-options-set/.code = \def\@bohr@electron@options{#1} ,
    electron-options-add/.code =
      \expandafter\def\expandafter\@bohr@electron@options\expandafter{\
@bohr@electron@options,#1} ,
    shell-dist/.code           = \def\@bohr@shell@dist{#1} ,
    shell-options-set/.code    = \def\@bohr@shell@options{#1} ,
```

```
    shell-options-add/.code    =
      \expandafter\def\expandafter\@bohr@shell@options\expandafter{\
  @bohr@shell@options,#1} ,
    german/.is if              = bohr@german ,
    ngerman/.is if             = bohr@german
}

\newrobustcmd\setbohr[1]{\pgfqkeys{/bohr}{#1}}

\ProcessPgfOptions*
\endinput

% HISTORY
2012/09/21 v0.1a - first version on bitbucket
2012/09/22 v0.2  - added compatibility up to atomic number 112
                 - added the commands \elementname and \elementsymbol with
                   language support German and English
                 - improved error checking
```

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