BOHR

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simple atom representation according to the Bohr model

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English documentation

This package provides means for the creation of simple Bohr models of atoms up to the atomic number 54. It 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] and etoolbox.[2]

2 Usage

BOHR is used like any other LaTeX 2ε package:

```
\usepackage{bohr}
```

It has no options so that's it.

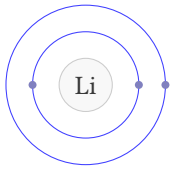
BOHR provides a single command, \bohr, which creates the models:

[1] CTAN: tikz [2] CTAN: etoolbox

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

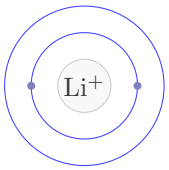
This is described best by an example:

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



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

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



3 Customization

BOHR provides a few options to customize the appearance:

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

▸ `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`.

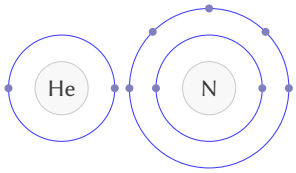
▸ `electron-radius = <dim>` Default: `1.5pt`
The radius of the circles that represent the electrons.

▸ `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.

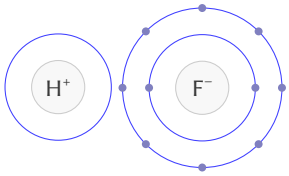
▸ `shell-options-add = <tikz>` (initially empty)
This value will be added to options set with `shell-options-set`.

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

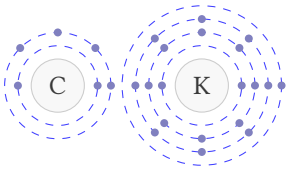
```
\setbohr{name-options-set={font=\footnotesize\sffamily}}
\bohr{2}{He} \bohr{7}{N}
```




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




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



4 Implementation

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

% the BOHR package
%
%   simple atom representation according to the Bohr model
%
% ------------------------------------------------------------------------------

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% 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 and README
% ------------------------------------------------------------------------------

% If you have any ideas, questions, suggestions or bugs to report, please
% feel free to contact me.
% ------------------------------------------------------------------------------

\def\@bohr@date{2012/09/21}
\def\@bohr@version{0.1a}
\def\@bohr@description{simple atom representation according to the Bohr
  model}

\ProvidesPackage{bohr}[\@bohr@date\space \@bohr@version\space \
  @bohr@description]
\RequirePackage{tikz,etoolbox}

\newrobustcmd*\bohr[3][]{\@bohr{#1}{#2}{#3}}

```

```
\def\@bohr#1#2#3{%
  \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 use \@bohr@shell@num\space shells.}%
      \else
        \def\@bohr@shell@num{#1}%
      \fi
    }%
  \tikzpicture[baseline=(nucleus.base)]
    \expandafter\node\expandafter[\@bohr@name@options]
      (nucleus) at (0,0) {\@bohr@write@atom{#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
            \@bohr@error{I don't know how to draw #1 electrons!}%
          \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}%
            \fi
          \fi
        \fi
      \fi
    \fi
  \fi
}
```

```
134
135 % definable parameters:
136 \def\@bohr@name@options{}
137 \def\@bohr@write@atom#1{#1}
138 \def\@bohr@nucleus@radius{1em}
139 \def\@bohr@electron@options{blue!50!black!50}
140 \def\@bohr@electron@radius{1.5pt}
141 \def\@bohr@shell@dist{1em}
142 \def\@bohr@nucleus@options{draw=black!80,fill=black!10,opacity=.25}
143 \def\@bohr@shell@options{draw=blue!75,thin}
144
145 \pgfkeys{
146   bohr/.cd,
147     atom-style/.code           = \def\@bohr@write@atom{#1} ,
148     name-options-set/.code     = \def\@bohr@name@options{#1} ,
149     name-options-add/.code     =
150       \expandafter\def\expandafter\@bohr@name@options\expandafter{\
  @bohr@name@options,#1} ,
151     nucleus-radius/.code       = \def\@bohr@nucleus@radius{#1} ,
152     nucleus-options-set/.code  = \def\@bohr@nucleus@options{#1} ,
153     nucleus-options-add/.code  =
154       \expandafter\def\expandafter\@bohr@nucleus@options\expandafter{\
  @bohr@nucleus@options,#1} ,
155     electron-radius/.code      = \def\@bohr@electron@radius{#1} ,
156     electron-options-set/.code = \def\@bohr@electron@options{#1} ,
157     electron-options-add/.code =
158       \expandafter\def\expandafter\@bohr@electron@options\expandafter{\
  @bohr@electron@options,#1} ,
159     shell-dist/.code           = \def\@bohr@shell@dist{#1} ,
160     shell-options-set/.code    = \def\@bohr@shell@options{#1} ,
161     shell-options-add/.code    =
162       \expandafter\def\expandafter\@bohr@shell@options\expandafter{\
  @bohr@shell@options,#1}
163 }
164
165 \newrobustcmd\setbohr[1]{\pgfqkeys{/bohr}{#1}}
166
167 \def\@bohr@error#1{\PackageError{bohr}{#1}{}}
168 \def\@bohr@warning#1{\PackageWarning{bohr}{#1}{}}
169 \endinput
170
171 % HISTORY
172 2012/09/21 v0.1a - first version on bitbucket
```

Index