BOHR

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simple atom representation according to the Bohr model

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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?

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1 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."

The BOHR package loads and needs the packages pgf[1] [Tan13], pgfopts[2] [Wri11], elements[3] [Nie15] and cnltx-base[4] [Nie14].

1. on CTAN as pgf: http://mirrors.ctan.org/graphics/pgf/
2. on CTAN as pgfopts: http://mirrors.ctan.org/macros/latex/contrib/pgfopts/
3. on CTAN as elements: http://mirrors.ctan.org/macros/latex/contrib/elements/
4. on CTAN as cnltx: http://mirrors.ctan.org/macros/latex/contrib/cnltx/

2 News

With version 1.0 all the parts not directly used for drawing the Bohr models such as defining element names (\setatomname) or element symbols (\setatomsymbol) or writing the electron configuration (\elconf) have been extracted into a new package called elements. This package provides all the commands besides \bohr and \setbohr that you know from earlier versions of BOHR. As a consequence the option language has been dropped. Obviously said package is now needed by BOHR.

3 Options

Every option described in the manual can also be used as package option although this is not really advertised. The preferred version is to set options via the setup command \setbohr. Future versions of \bohr may drop the possible package options completely. Options are indicated as option and are all key/value like options. Some options can be set without value, too. Then the underlined value is used.

4 Usage

BOHR is used like any other LaTeX 2ε package:

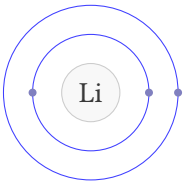
```
1 \usepackage{bohr}
```

The main command, \bohr, creates the models:

\bohr[⟨*num of shells*⟩]{⟨*num of electrons*⟩}{⟨*atom name*⟩}
The main command. The mandatory arguments take the number of electrons to be printed and the atom symbol that is printed in the center.

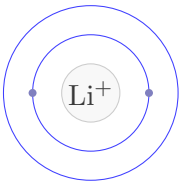
This is described best by an example:

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



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

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



5 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` = `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.

`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` Default: `false`
Sets both `insert-symbol` and `insert-number`.

`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 option*⟩} (initially empty)
This value is passed to the options of the `\node` the third argument of `\bohr` is placed in.

`name-options-add` = {⟨*tikz options*⟩} (initially empty)
This value will be added to options set with `name-options-set`.

`nucleus-options-set` = {⟨*tikz options*⟩}
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 options*⟩} (initially empty)
This value will be added to options set with `nucleus-options-set`.

`nucleus-radius` = {⟨*dimension*⟩} Default: `1em`
The radius of the circle around the name-node.

`electron-options-set` = {⟨*tikz options*⟩} Default: `blue!50!black!50`
This value is passed to the options of the `\fill` command that draws the electrons.

`electron-options-add` = {⟨*tikz options*⟩} (initially empty)
This value will be added to options set with `electron-options-set`.

`electron-radius` = {⟨*dimension*⟩} Default: `1.5pt`
The radius of the circles that represent the electrons.

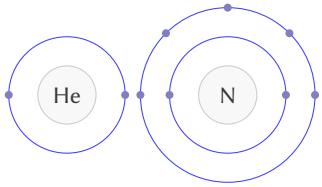
`shell-options-set` = {⟨*tikz options*⟩} Default: `draw=blue!75,thin`
This value is passed to the options of the `\draw` command that draws the circles that represent the shells.

`shell-options-add` = {⟨*tikz options*⟩} (initially empty)
This value will be added to options set with `shell-options-set`.

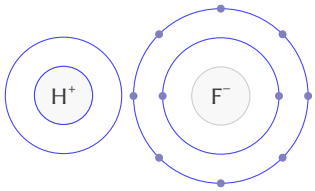
`shell-dist` = {⟨*dimension*⟩} Default: `1em`
The distance between the nucleus and the first shell and between subsequent shells.

`distribution-method` = `periodic|quantum` Default: `quantum`
Introduced in version 0.3
Determines how the electrons are distributed on the shells. `periodic` distributes the electrons 2-8-8-18-18-32-32, *i. e.*, according to the place of the corresponding atom in the periodic table of elements. `quantum` distributes the electrons according to the electron configuration of the corresponding atom where each shell represents the main quantum number. Pd for example has the configuration $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10}$ and would get two electrons on the first shell, 8 electrons on the second, and 18 electrons each on the third and fourth.

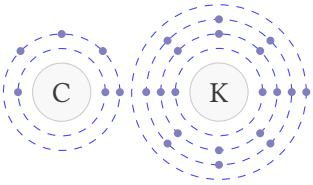
```
\setbohr{name-options-set={font=\footnotesize\sffamily}}
\bohr{2}{He} \bohr{7}{N}
```




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

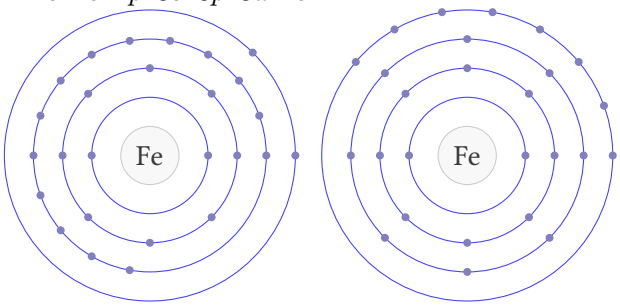



```
\setbohr{
  shell-options-add = dashed,
  shell-dist        = .5em,
  insert-missing
}
\bohr{6}{} \bohr{}{K}
```




```
\setbohr{distribution-method=quantum,insert-missing}
\elconf{Fe} \\ % provided by `elements'
\bohr{}{Fe}
\setbohr{distribution-method=periodic}
\bohr{}{Fe}
```

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2$



References

[Nie14] Clemens Niederberger. cnltx. version 0.10a, Jan. 23, 2014. URL: http://mirror.ctan.org/macros/latex/contrib/cnltx/.

[Nie15] Clemens Niederberger. elements. version 0.1, June 14, 2015. URL: http://mirror.ctan.org/macros/latex/contrib/elements/.

[Tan13] Till Tantau. TikZ/pgf. version 3.0.0, Dec. 13, 2013.
URL: http://mirror.ctan.org/graphics/pgf/.

[Wri11] Joseph Wright. pgfopts. version 2.1, June 2, 2011.
URL: http://mirror.ctan.org/macros/latex/contrib/pgfopts/.

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