CARBOHYDRATES

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carbohydrate molecules with chemfig

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CARBOHYDRATES offers macros for making exercise sheets when teaching carbohydrate chemistry a lot less tedious. It uses chemfig for drawing the formulas.

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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."

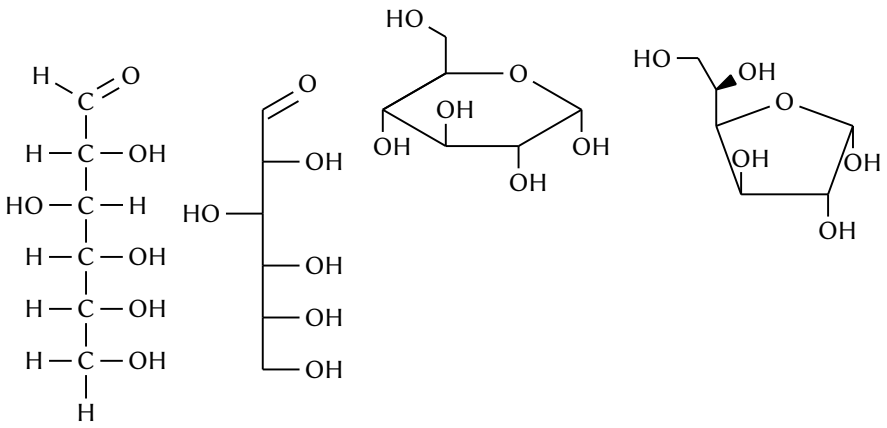
CARBOHYDRATES loads the packages chemfig [Tel15], etoolbox [Leh15] and xcolor [Ker07].

2 The Idea

When teaching chemistry – and in the case of this package: carbohydrate chemistry – you have to show many examples of the basic aldoses and you have to explain the Fischer and the Haworth representation as well. This means you may have nearly the same chemfig [Tel15] formulas over and over in your documents. CARBOHYDRATES aims to ease this task.

The following example will give a short impression of what the package does:

```
\glucose
\glucose[model={fischer=skeleton}]
\setatomsep{2.5em}
\glucose[model=haworth,ring]
\glucose[model=haworth,ring=furanose]
```



3 Usage

3.1 The Base Macro

`\carbohydrate[`⟨*options*⟩`]{`⟨*spec*⟩`}`

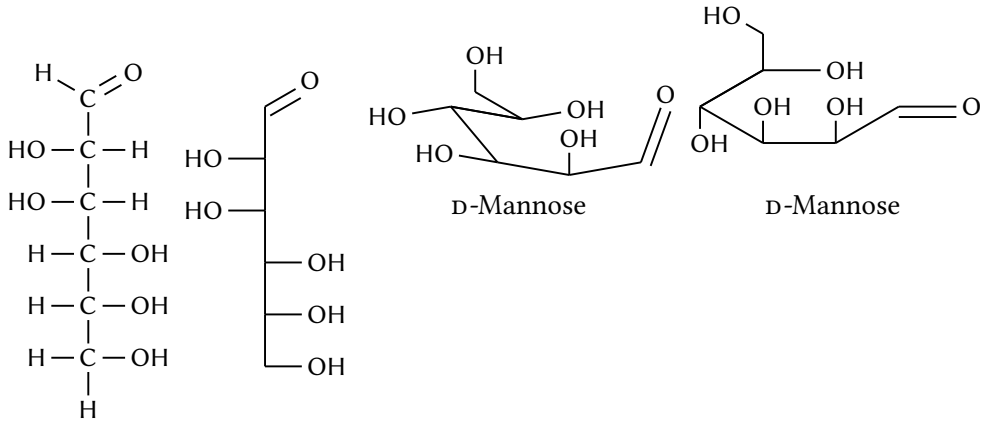
A generic macro for typesetting carbohydrates.

We will talk about the options in a bit. First lets see what ⟨*spec*⟩ means. This argument is a series of the tokens `r`, `l` and `0` denoting an hydroxy group placed to the right or the left in the Fischer projection of the carbohydrate. A `0` means that the hydroxy group is to be left out. The series of tokens is meant to describe the hydroxy groups at the chiral centers. The aldehyde group[1] and the hydroxy group at the end of the chain will be set automatically. Unless specified otherwise the command expects a hexose which means a series of *four* tokens.

```
\chemname{\carbohydrate{llrr}}{\iupac{\D-Mannose}}
\chemname{\carbohydrate[model={fischer=skeleton}]{llrr}}{\iupac{\D-Mannose}}
\setatomsep{2.5em}\chemnameinit{}
\chemname{\carbohydrate[model=chair]{llrr}}{\iupac{\D-Mannose}}
```

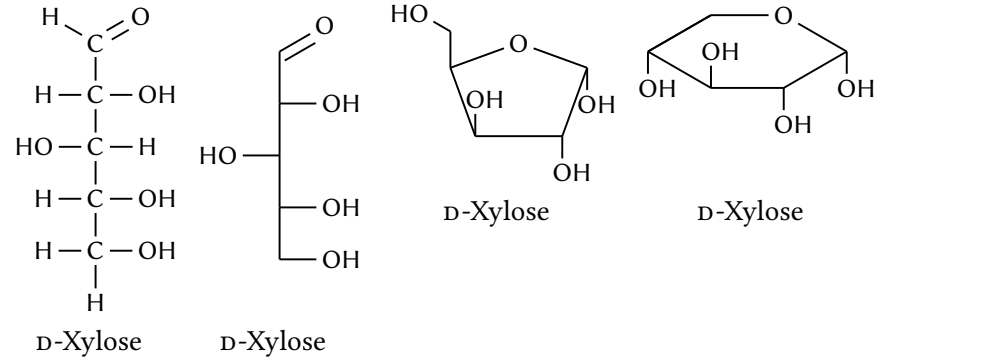
1. Also the keto group once ketoses will be implemented.

```
\chemname{\carbohydrate[model=haworth]{llrr}}{\iupac{\D-Mannose}}
```



Adding the option `pentose` means that now only *three* tokens need to be specified.

```
\chemname{\carbohydrate[pentose]{rlr}}{\iupac{\D-Xylose}}
\chemname{\carbohydrate[pentose,model={fischer=skeleton}]{rlr}}{\iupac{\D-Xylose}}
\setatomsep{2.5em}\chemnameinit{}
\chemname{\carbohydrate[pentose,model=haworth,ring]{rlr}}{\iupac{\D-Xylose}}
\chemname{\carbohydrate[pentose,model=haworth,ring=pyranose]{rlr}}{\iupac{\D-Xylose}}
```



3.2 Available Options

As you have already seen in the pevious examples `\carbohydrate` has an optional argument that takes different options. Here is a complete list:

`model` = `fischer|haworth|chair` Default: `fischer`
The model to be used to draw the molecule. The choice `fischer` is itself an option with two choices: `fischer` = `{skeleton}` and `fischer` = `{full}`. Leaving the choice out will use `full` as default choice.

`chain`
Draw the open chain isomer.

`ring` = `true|pyranose|furanose`
Draw a ring isomer. If you don't specify what ring type should be drawn (*i. e.*, if you choose `true`) the default depends on the length of the carbohydrate. For example for hexoses the default ring type is `pyranose`.

`anomer` = `alpha|beta|undetermined` Default: `alpha`
The ring anomer.

`length` = `6|5|4|3` Default: `6`
The length of the carbohydrate. `length` = `{6}` draws a hexose, `length` = `{3}` draws a triose.

`hexose`
An alias for `length` = `{6}`.

`pentose`
An alias for `length` = `{5}`.

`tetrose`
An alias for `length` = `{4}`.

`triose`
An alias for `length` = `{3}`.

`3d` = `true|false` Default: `false`
Draw some of the bonds of the rings in the `haworth` and `chair` models in a way that indicates the three dimensional structure of the molecules.

`color` = `{`⟨*name*⟩`}{`⟨*color*⟩`}`
This option takes two arguments: ⟨*name*⟩ specifies which part of the molecule is to be colored, ⟨*color*⟩ specifies the color to be used, also see table 1 on the following page and section 3.7.

3.3 Defining Shortcuts

CARBOHYDRATES allows to define shortcuts for aldoses:

`\newaldose{`⟨*cs*⟩`}[`⟨*options*⟩`]{`⟨*spec*⟩`}`
This defines the macro ⟨*cs*⟩ with preset options ⟨*options*⟩. ⟨*spec*⟩ has the same meaning as for `\carbohydrate`.

TABLE 1: Available names for the color option.

Name	Function
C1	carbon 1
C2	carbon 2
O-C2	oxygen of the hydroxy group at carbon 2
H-C2	hydrogen of the hydroxy group at carbon 2
C3	carbon 3
O-C3	oxygen of the hydroxy group at carbon 3
H-C3	hydrogen of the hydroxy group at carbon 3
C4	carbon 4
O-C4	oxygen of the hydroxy group at carbon 4
H-C4	hydrogen of the hydroxy group at carbon 4
C5	carbon 5
O-C5	oxygen of the hydroxy group at carbon 5
H-C5	hydrogen of the hydroxy group at carbon 5
C6	carbon 6
O-C6	oxygen of the hydroxy group at carbon 6
H-C6	hydrogen of the hydroxy group at carbon 6
anomerO	oxygen of the anomeric hydroxy group/aldehyde oxygen
anomerH	hydrogen of the anomeric hydroxy group
ringO	oxygen in the ring

`\renewaldose{`⟨*cs*⟩`}[`⟨*options*⟩`]{`⟨*spec*⟩`}`
The same command but redefines an existing macro.

In fact, CARBOHYDRATES already defines macros for the common aldoses. They are listed in table 2 on page 6. They don't have any predefined options (except for hexose, pentose *etc.*).

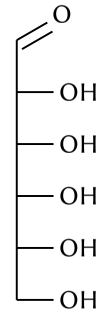
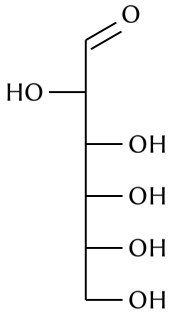
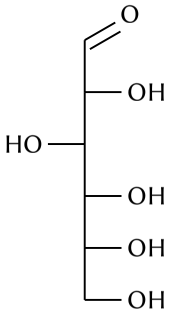
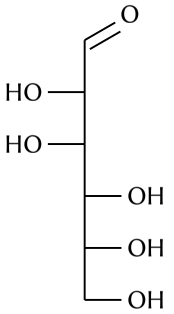
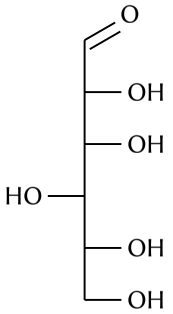
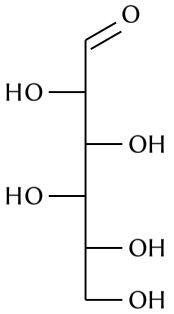
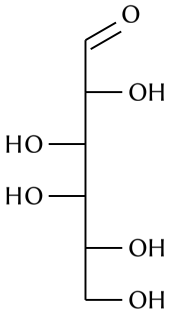
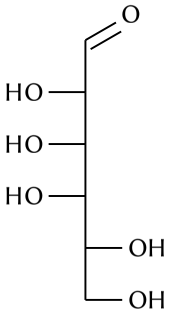
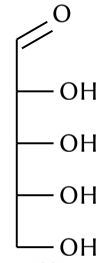
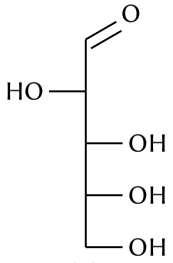
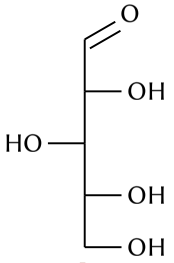
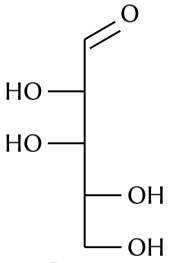
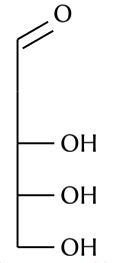
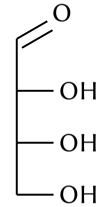
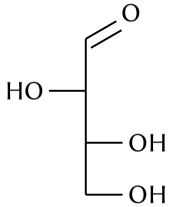
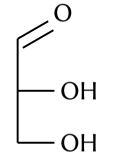
3.4 Available Models

CARBOHYDRATES implements different models for drawing carbohydrates:

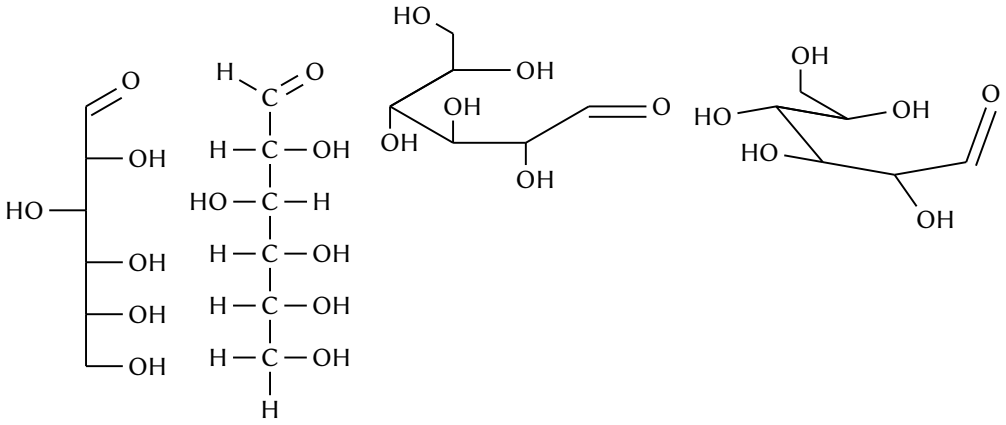
- Fischer – skeleton: the Fischer representation with only a skeleton formula.
- Fischer – full: the Fischer representation including all C and H atoms.
- Haworth: the Haworth representation.
- Chair: the chair conformation.

While the Fischer model is implemented for all carbohydrates both Haworth and chair are not. The chair model is only implemented for aldohexoses, Haworth is implemented for aldotetroses, -pentoses and -hexoses.

Table 2: Overview over the predefined aldoses.

 \allose D-Allose	 \altrose D-Altrose	 \glucose D-Glucose	 \mannose D-Mannose	 \gulose D-Gulose	 \idose D-Idose	 \galactose D-Galactose	 \talose D-Talose
 \ribose D-Ribose	 \arabinose D-Arabinose	 \xylose D-Xylose	 \lyxose D-Lyxose	 \desoxyribose D-Desoxy-ribose			
 \erythrose D-Erythrose	 \threose D-Threose	 \glycerinaldehyde D-Glycerin-aldehyde					

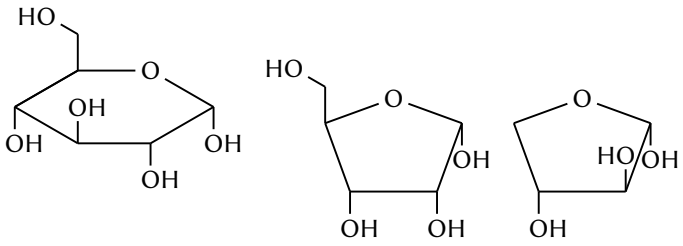
```
\glucose[model={fischer=skeleton}]
\glucose[model={fischer=full}]
\setatomsep{2.5em}
\glucose[model=haworth]
\glucose[model=chair]
```



3.5 Chain *vs.* Ring Forms

While the chain forms are available in all models the ring forms obviously aren't. There are two ring forms for hexoses and pentoses: pyranoses and furanoses. For tetroses only the furanose rings are available as there don't exist pyranose ring forms (for obvious reasons). It is also clear that neither pyranose nor furanose forms of trioses exist.

```
\setatomsep{2.5em}
\glucose[model=haworth,ring]
\ribose[model=haworth,ring]
\threose[model=haworth,ring]
```



Actually the above is not true: the chain forms are not available in all models for all

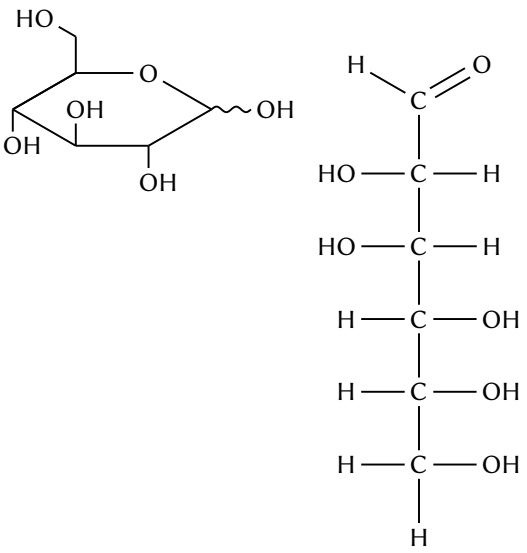
aldoses. As said in section 3.4 the chair model is only implemented for aldohexoses. Also chains are not implemented for tetroses and trioses in the Haworth model.

3.6 Default Settings

`\setcarbohydrate{`⟨*options*⟩`}`
Set package options for all carbohydrates within the current scope.

`\setcarbohydratedefaults{`⟨*csname*⟩`}{`⟨*options*⟩`}`
Set options for a predefined carbohydrate within the current scope. The first argument ⟨*csname*⟩ is the macro name of the shortcut (see section 3.3).

```
\setatomsep{2.5em}
\setcarbohydratedefaults\glucose{ring,model=haworth,anomer=undetermined}
\glucose\
\mannose
```

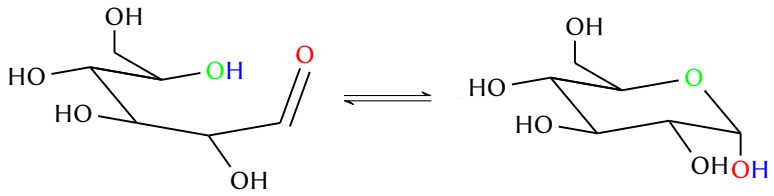


3.7 Colors

For educating purposes it may be useful to be able to color certain atoms. The `color` option allows this.

```
\setcarbohydrates{model=chair}
\setatomsep{2.5em}
```

```
\schemestart
  \glucose[color={anomerO}{red},color={O-C5}{green},color={H-C5}{blue}]
  \arrow{<=>}
  \glucose[ring,color={anomerO}{red},color={ringO}{green},color={anomerH}{blue
  }]
\schemestop
```



4 TODOS

There are still quite a number of missing features that I'd like to implement some day such as

- ring forms for L-carbohydrates,
- support for both chair conformations and the boat conformation,
- support for ketoses,
- support for oxidized and reduzed forms, and
- disaccharides.

There is *no* time table, though – wether these features will be implemented any time soon or at all is undecided.

5 About the Examples in this Manual

All macros used in the examples either belong to CARBOHYDRATES and are described in this manual or they belong to either chemfig [Tel15], chemmacros [Nie15b], chemformula [Nie15a], or are standard LaTeX macros. I encourage you to take a look at the packages for typesetting chemistry documents.

The chemfig settings have been adjusted for the examples in this manual. Specifically the preamble of this document makes these settings:

```
\newcommand*{\bondwidth}{0.06642 em}
\newcommand*{\bondboldwidth}{0.22832 em}
\newcommand*{\bondhashlength}{0.25737 em}
\setdoublesep{0.35700 em}
\setatomsep{1.78500 em}
```

```
\setbondoffset{0.18265 em}
\setbondstyle{line width = \bondwidth}
\setcrambond
  {\dimexpr\bondwidth*2 + \bondboldwidth\relax}
  {\bondwidth}
  {\bondhashlength}
\renewcommand*\printatom[1]{{\small\ensuremath{\mathsf{#1}}}}
```

These settings are taken from [Wri]. Search the page for `chemfig` and you should be able to find them there.

References

[Ker07] Uwe Kern. xcolor. version 2.11, Jan. 21, 2007.
URL: http://mirror.ctan.org/macros/latex/contrib/xcolor/.

[Leh15] Philipp Lehman, current maintainer: Joseph Wright.
etoolbox. version 2.2a, Aug. 2, 2015.
URL: http://mirror.ctan.org/macros/latex/contrib/etoolbox/.

[Nie15a] Clemens Niederberger. chemformula. version 4.11, June 30, 2015.
URL: http://mirror.ctan.org/macros/latex/contrib/chemformula/.

[Nie15b] Clemens Niederberger. chemmacros. version 5.2, Oct. 14, 2015.
URL: http://mirror.ctan.org/macros/latex/contrib/chemmacros/.

[Tel15] Christian Tellechea. chemfig. version 1.2c, Nov. 20, 2015.
URL: http://mirror.ctan.org/macros/generic/chemfig/.

[Wri] Joseph Wright. URL: http://www.texdev.net/ (visited on 04/25/2014).

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