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 formulae.

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1 Licence and Requirements

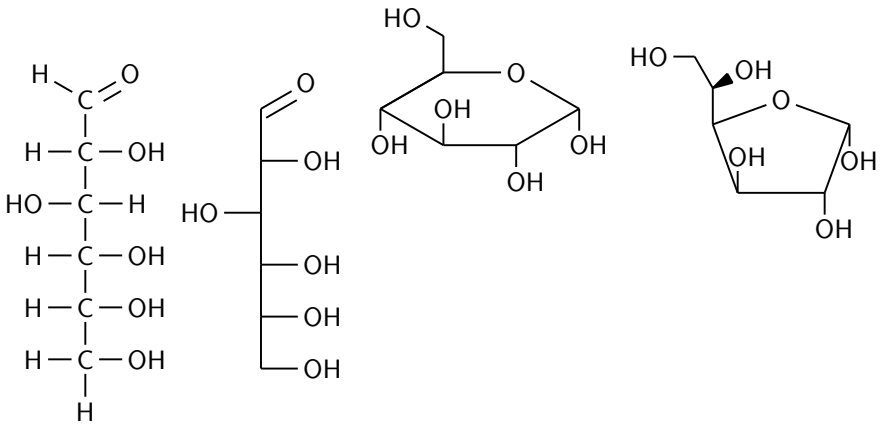
CARBOHYDRATES loads the packages chemfig [Tel13] and cnltx-base, the programming package fom the cnltx bundle [Nie14b].

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 formulae 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

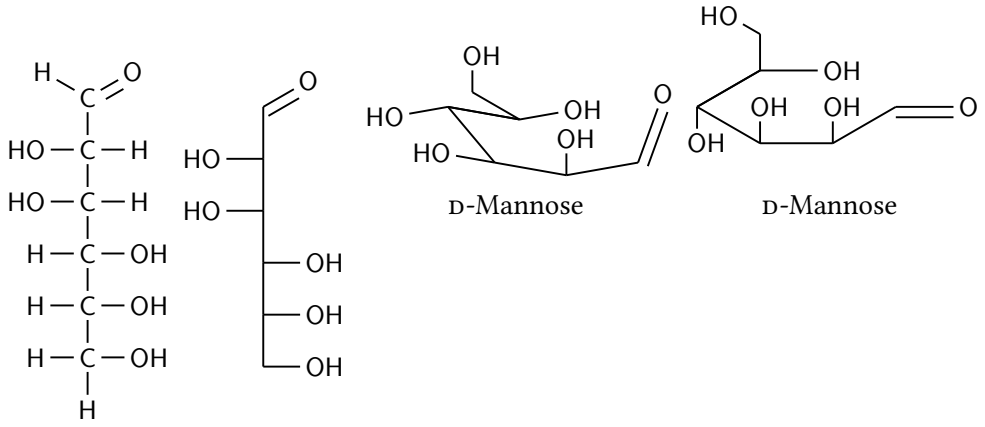
`\carbohydrate[`⟨*options*⟩`]{`⟨*spec*⟩`}`

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 thet 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 hydrohy group at the end of the molecule will be set automatically. Unless specified otherwise the command expects a hexose which means a series of *four* tokens.

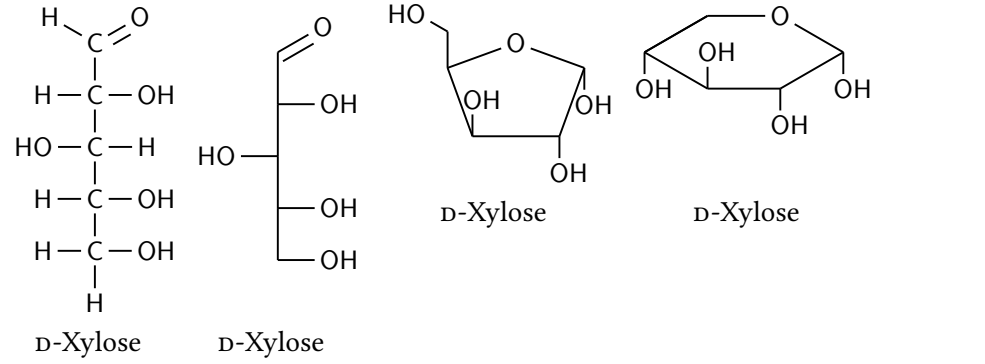
```
\chemname{\carbohydrate{llrr}}{\iupac{\D-Mannose}}
\chemname{\carbohydrate[model={fischer=skeleton}]{llrr}}{\iupac{\D-Mannose}}
\setatomsep{2.5em}\chemnameinit{}
\chemname{\carbohydrate[model=chair]{llrr}}{\iupac{\D-Mannose}}
\chemname{\carbohydrate[model=haworth]{llrr}}{\iupac{\D-Mannose}}
```

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



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 draw (*i. e.*, if you choose `true`) the default depends on the length of the carbohydrate. Ror 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` in a way that indicates the three dimensional structure of the molecules.

3.3 Defining Shortcuts

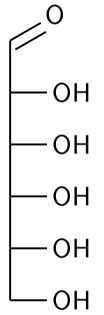
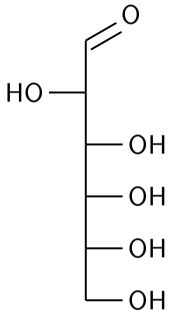
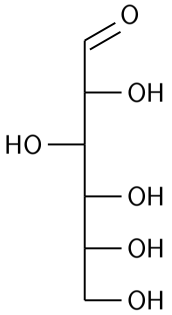
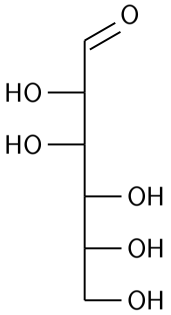
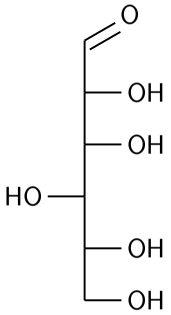
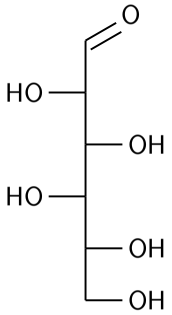
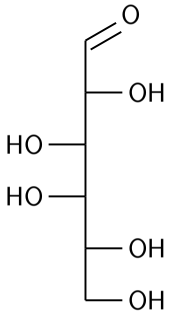
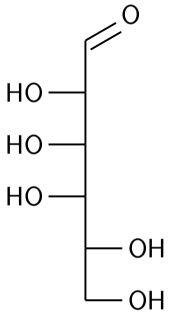
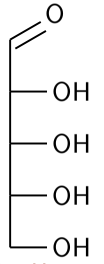
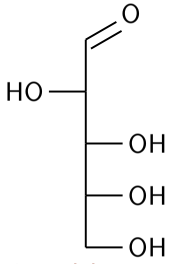
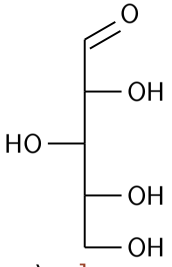
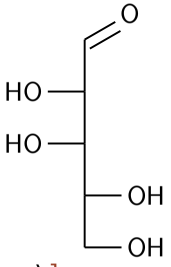
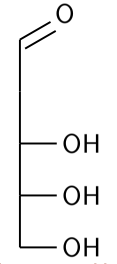
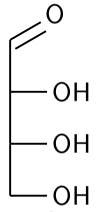
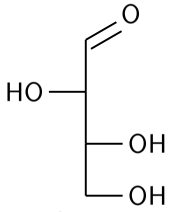
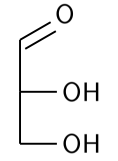
CARBOHYDRATES allows to define shortcuts for aldoses:

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

`\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 1 on page 5. They don't have any predefined options (except for `hexose`, `pentose` *etc.*).

Table 1: 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					

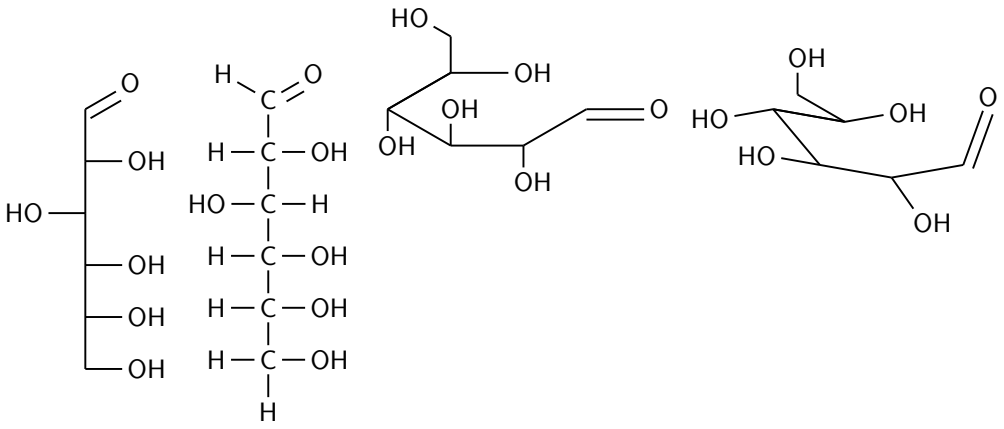
3.4 Available Models

CARBOHYDRATES implements different models how to draw 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.

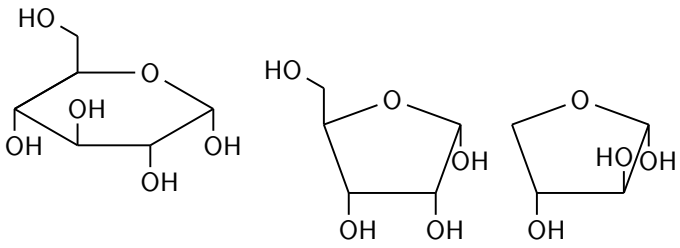
```
\glucose[model={fischer=skeleton}]
\glucose[model={fischer=full}]
\setatomsep{2.5em}
\glucose[model=haworth]
\glucose[model=chair]
```



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]
```

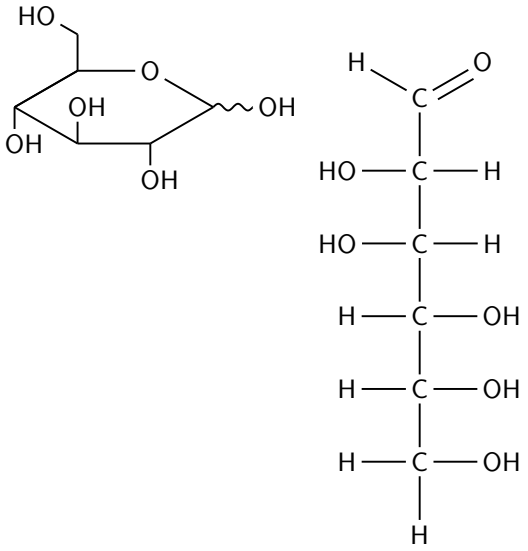


3.6 Default Settings

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

`\setcarbohydratedefaults{`⟨*csname*⟩`}{`⟨*options*⟩`}`
Set options for a predefined carbohydrate. The first argument ⟨*csname*⟩ is the macro name of the shortcut (see section 3.3) *without* leading backslash.

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



4 Restrictions and TODOs

4.1 TODOs

There are still a number of missing features that I plan to implement someday such as:

- ring forms for L-carbohydrates,
- support for ketoses and
- support for oxidized and reduzed forms.

5 About the Examples

All macros used in the examples either belong to CARBOHYDRATES and are described in this manual or they belong to either chemfig or chemmacros [Nie14a].[2] I encourage you to take a look at those packages if you don't know them already.

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
  {\the\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

[Nie14a] Clemens NIEDERBERGER. chemmacros. version 4.3, Jan. 24, 2014. URL: http://mirror.ctan.org/macros/latex/contrib/chemmacros/.

[Nie14b] Clemens NIEDERBERGER. cnltx. version 0.10a, Jan. 23, 2014. URL: http://mirror.ctan.org/macros/latex/contrib/cnltx/.

[Tel13] Christian TELLECHEA. chemfig. version 1.0h, Nov. 28, 2013. URL: http://mirror.ctan.org/macros/generic/chemfig/.

2. That is if they're not standard LaTeX macros.

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

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