QUELQUES PACKAGES COMPLÉMENTAIRES DE CHIMIE

Ce document nécessite de connaître les bases de LaTeX, Ti*k*z et ChemFig

1–Package `chemmacros`

1.1–Commandes diverses

```
\Hpl \Hyd \HtO \water
\el \prt \ntr
\delp \delm \scrp \scrm
\fplus \fminus
\Rconf \Rconf[] \Sconf \Rconf[]
\pH \pOH \Ka \Kb \Kw \Ka \Kb \pKa \pKa[1] \pKb \pKb[1]
```

H^+ OH^- H_3O^+ H_2O

e^- p^+ n^0

$\delta+$ $\delta-$ $+$ $-$

⊕ ⊖

(R) ↻ (S) ↻

pH pOH K_A K_B K_W K_A K_B pK_A pK_{A1} pK_B pK_{B1}

1.2–Oxydo-réduction

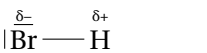
```
\leavevmode
\pch, Na\pch, Ca\pch[2]
\mch, F\mch, S\mch[2]
\fpch\ \fmch\ \fpch[3] \fmch[3]
```

$^+$, Na^+, Ca^{2+}
$^-$, F^-, S^{2-}
⊕ ⊖ 3⊕ 3⊖

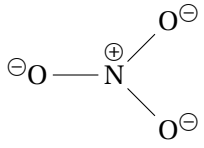
```
\chemsetup{ox/parse= false}
\ox{+1,Na} \ox{2,Ca} \ox{-2,S} \ox{-1,F} \ox[pos=super]{3,Fe} \ox[pos=side]{3,Fe}
```

$\overset{+1}{Na}$ $\overset{2}{Ca}$ $\overset{-2}{S}$ $\overset{-1}{F}$ Fe^3 Fe(3)

```
\chemsetup{ox/parse= false}
\chemfig{\chemabove[3pt]{\lewis{246,Br}}{\delm}-\chemabove[3pt]{H}{\delp}}
```



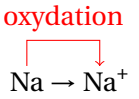
```
\chemfig{\fmch{}|O-\chemabove{N}{\fscrp}(-[1]O|\fmch)-[7]O|\fmch}
```

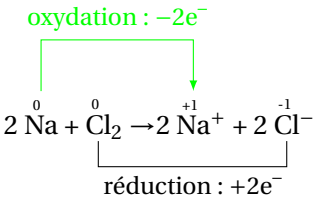


```
\OX{a,Na} $\rightarrow$ \OX{b,Na}\pch
\redox(a,b)[->,red]{oxydation}

2 \OX{o1,\ox{0,Na}} + \OX{r1,\ox{0,Cl}}$_2$ $\rightarrow$
```

```
2 \OX{o2,\ox{+1,Na}}$^+$ + 2 \OX{r2,\ox{-1,Cl}}$^-$
\redox(o1,o2){\small oxydation: $- 2\el$}
\redox(r1,r2)[][-1]{\small réduction: $+ 2\el$}
```






```
\chemsetup[phases]{pos=sub}
\ch{C\sld{} + 2 H2O\lqd{} -> CO2\gas{} + 2 H2\gas}\par
 NaCl\aq\\
 \ch{H2O "\lqd[\SI{5}{\celsius}]"}
```

$C_{(s)} + 2\,H_2O_{(l)} \longrightarrow CO_{2(g)} + 2\,H_{2(g)}$

$NaCl_{(aq)}$
$H_2O_{(l)}[5\,°C]$

1.3–Alignement des équations

L'environnement reactions* permet de ne pas avoir de label(compteur) après chaque équation.

```
\begin{reactions}
A &-> B + C \\
D + E &-> F
\end{reactions}

\begin{reactions}
A &-> B + C \\
D + E &-> F
\end{reactions}

\begin{reactions}
A + 2 B &-> 3 C + D \\
\intertext{Some text in between aligned reactions}
3 E + F &<=> G + 1/2 H
\end{reactions}
```

$$A \longrightarrow B + C \quad \{1\}$$
$$D + E \longrightarrow F \quad \{2\}$$

$$A + 2\,B \longrightarrow 3\,C + D \quad \{3\}$$
$$\{4\}$$

Some text in between aligned reactions

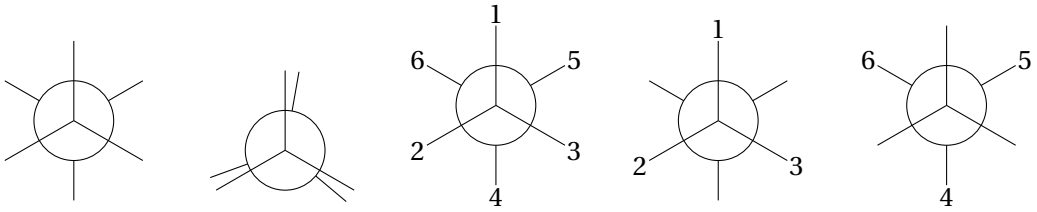
$$3\,E + F \rightleftharpoons G + \frac{1}{2}\,H \quad \{5\}$$

```
\renewtagform{reaction}[R \textbf]{[}{]}% personnalisation des labels
\begin{reaction}
H2O + CO2 <<=> H2CO3
\end{reaction}
```

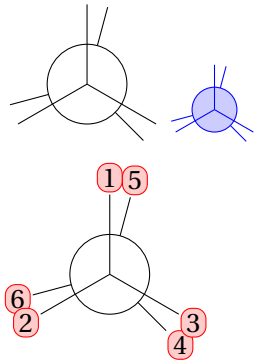
$$H_2O + CO_2 \rightleftharpoons H_2CO_3 \qquad [R\ \mathbf{6}]$$

1.4–Représentation de Newmann

```
\newman{}
\newman(170){}
\newman{1,2,3,4,5,6}
\newman{1,2,3}
\newman{,,,4,5,6}
```




```
\chemsetup[newman]{angle=45} \newman{}
\newman[scale=.75,ring={draw=blue,fill=blue!20}]{}
\chemsetup[newman]{atoms={draw=red,fill=red!20,inner sep=2pt,rounded corners}}
\newman{1,2,3,4,5,6}
```

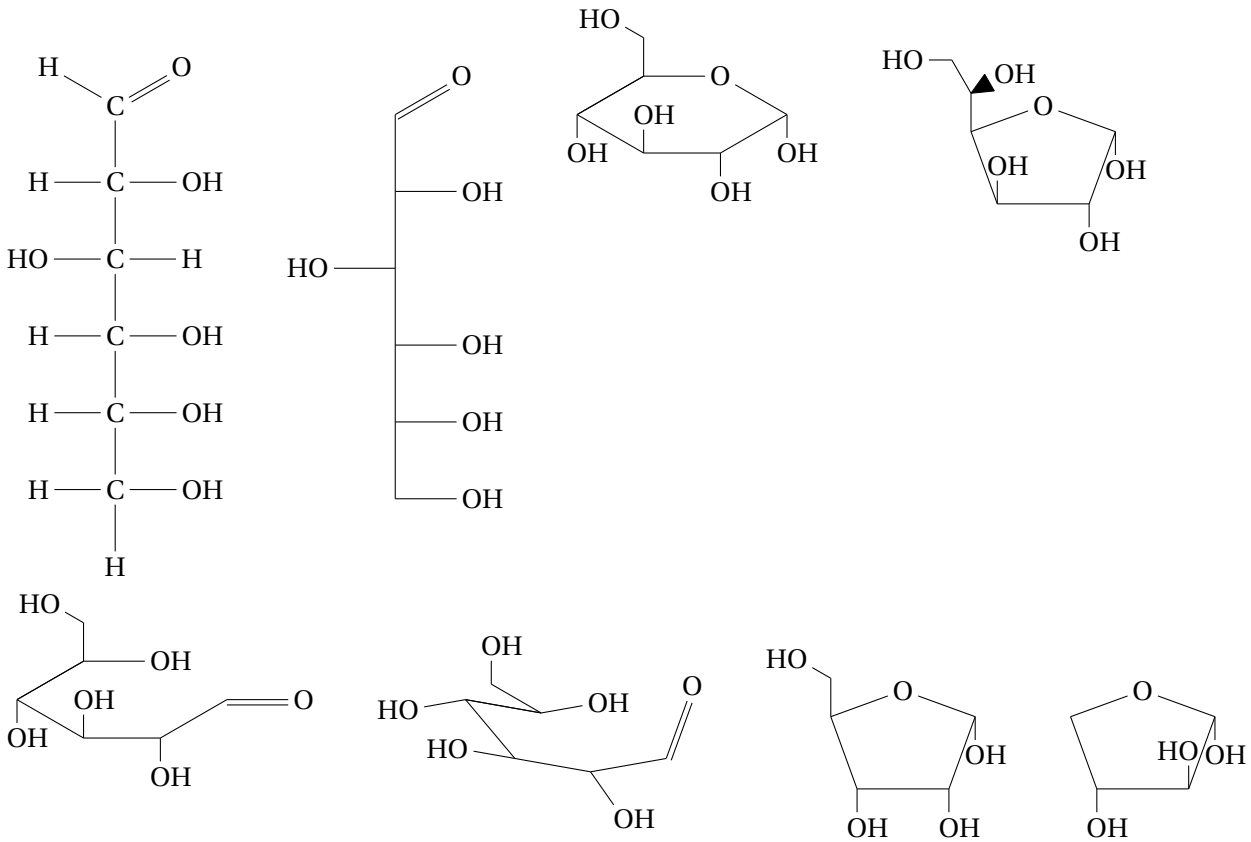


2–Package `carbohydrates`

Ce package charge aussi chemfig qui charge tikz.

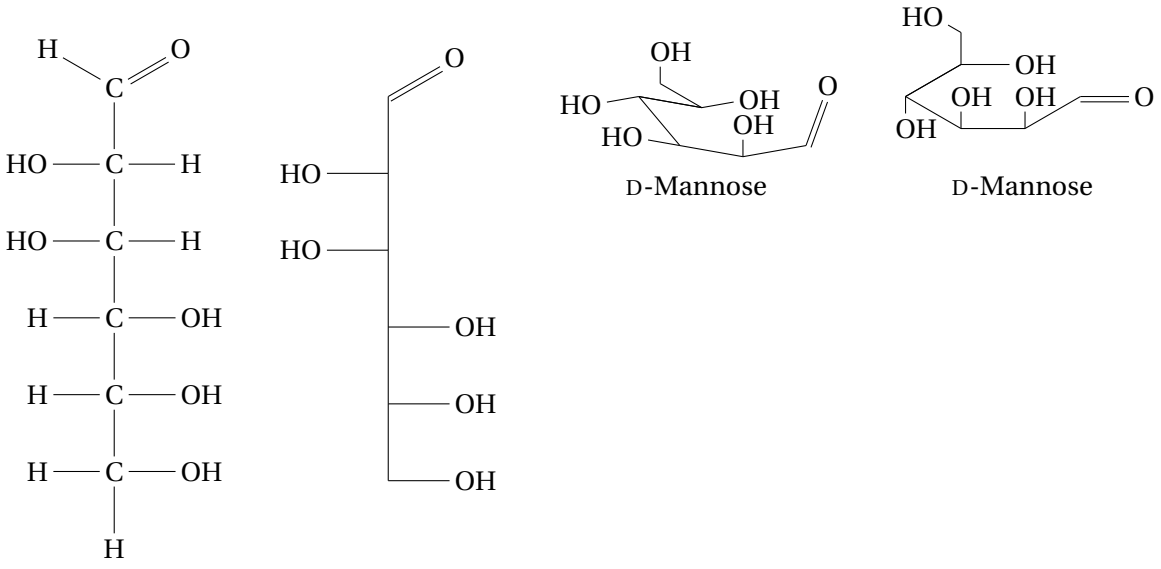
```
\glucose
\glucose[model={fischer=skeleton}]
\glucose[model=haworth,ring]
\glucose[model=haworth,ring=furanose]

\glucose[model=haworth]
\glucose[model=chair]
\ribose[model=haworth,ring]
\threose[model=haworth,ring]
```



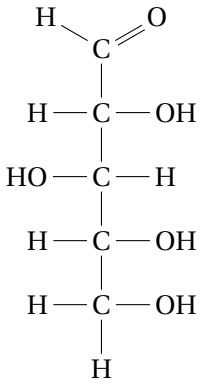
Il faut charger chemmacros :

```
\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}}
```

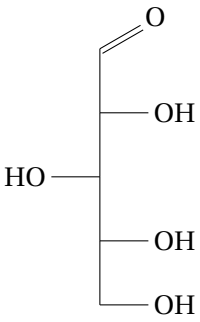


D-Mannose D-Mannose

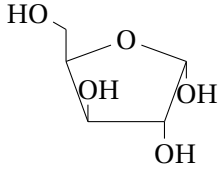
```
\chemname{\carbohydrate[pentose]{rlr}}{\iupac{\D-Xylose}}
\chemname{\carbohydrate[pentose,model={fischer=skeleton}]{rlr}}{\iupac{\D-
Xylose}}
\setatomsep{2.5em}\chemnameinit{}
\chemname{\carbohydrate[pentose,model=haworth,ring]{rlr}}{\iupac{\D-Xylose}}
\chemname{\carbohydrate[pentose,model=haworth,ring=pyranose]{rlr}}{\iupac{\D-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



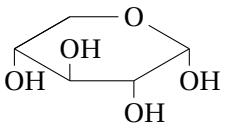
D-Xylose



D- Xylose



D-Xylose



D- Xylose

3–Police `emerald`

```
{\ECFAugie ChemFig}
```

ChemFig

Pour installer cette police sur Ubuntu, on peut procéder ainsi :

```
mkdir -p ‘kpsewhich --var-value=TEXMFHOME‘
cd ‘kpsewhich --var-value=TEXMFHOME‘
wget http://mirror.ctan.org/fonts/emerald.zip
unzip emerald.zip
cp -r emerald/. . && rm -rf emerald/
rm emerald.zip
updmap --enable Map emerald.map
texhash

%puis éventuellement:

mkdir -p ~/.texmf-config/web2c
echo Map emerald.map >> ~/.texmf-config/web2c/updmap.cfg
updmap
```