

CHEMFIG

Placer le package chemfig dans le préambule charge aussi le package tikz.

`\chemfig{<par défaut en mode mathématique sans mettre les balises $$$>`

1-Formules de Lewis

`\lewis{0246,A} \lewis{1357,B}`



`\lewis{0:2:4:6:,A} \lewis{0.2.4.6.,B} \lewis{0:2.4|,X} \lewis{5|7,0^+}` $\text{:}\ddot{\text{A}}\text{:}$ $\cdot\ddot{\text{B}}\cdot$ $\text{||}\ddot{\text{X}}\text{:}$ $\text{||}\text{O}^+\text{/}$

2-Types de liaisons

`\chemfig[<option de dessin>][<option sur atome>]{<code molécule>}`

<code>\chemfig{A-B}</code>	A — B	<code>\chemfig[line width=1.5pt]{A-B}</code>	A — B
<code>\chemfig{A~B}</code>	A ≡ B	<code>\chemfig{A>B}</code>	A ▶ B
<code>\chemfig{A<B}</code>	A ◀ B	<code>\chemfig[red]{A-B}</code>	A — B
<code>\chemfig{A<:B}</code>	A ⋯ B	<code>\chemfig[] [red]{A-B}</code>	A — B
<code>\chemfig{A< B}</code>	A ◁ B	<code>\chemfig[dashed,thick] [red]{A-B}</code>	A - - - B
<code>\chemfig{A=B}</code>	A = B	<code>\chemfig[] [rotate=30,scale=0.5]{A-B}</code>	A ↗
<code>\chemfig{A=B}</code>	A = B	<code>\chemfig{A^B}</code>	A = B

3-Angles

`<angle des liaisons>,<coefficient de longueur>,<numéro de l'atome de départ>,<numéro de l'atome d'arrivée>,<code tikz>`

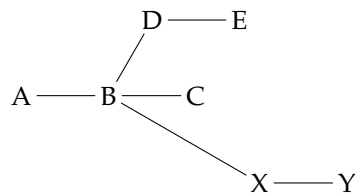
<code>\chemfig{A-B-[1]C-[2]D}\chemfig{--[1]-[2]}</code>	
<code>\chemfig{A-[:30]B=[:-75]C}</code>	
<code>\chemfig{A-[:-30]-[::+30]}</code>	
<code>\chemfig{ABCD-[:-60,,3,2]EFG}</code>	

Remarque : `\chemleft{\chemfig{A-[1]B}\chemright}` donne $\left[\begin{array}{l} \text{B} \\ \diagup \\ \text{A} \end{array} \right]$

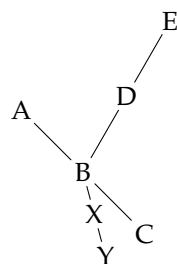
4-Ramifications

<code>\chemfig{A-B(-[1]W)(-[6]Y)-C}</code>	
--	--

`\chemfig{A-B(-[:60]D-E)(-[::-30,2]X-Y)-C}`

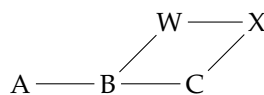


`\chemfig{[: -45]A-B[:60]-D-E([::-30,.5]-X-Y)-C}`

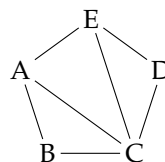


5-Cycles

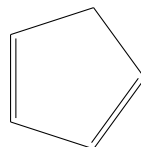
`\chemfig{A-B(-[1]W-X?)-C?}`



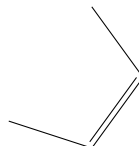
`\chemfig{A?[a]-[: -72]B-C?[a]?[b]-[:72]D-[:144]E?[a]?[b]}`



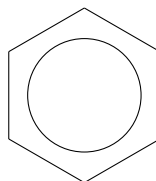
`\chemfig{*5(====)}`



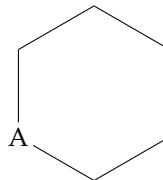
`\chemfig{*5(==)}`



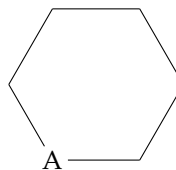
`\chemfig{*6(-----)}`



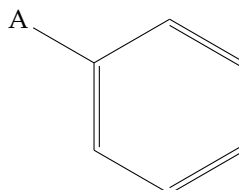
`\chemfig{A*6(-----)}`



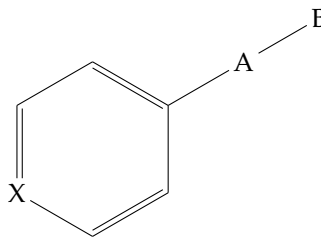
`\chemfig{[:30]A*6(-----)}`



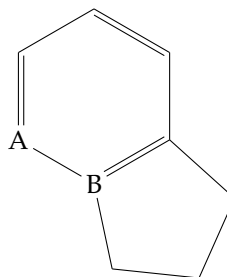
`\chemfig{A-[: -30]*6(====)}`



`\chemfig{X*6(---(-A-B)---)}`



`\chemfig{A*6(-B*5(-----)=====)}`



6-Modifications des distances, des espacements et autres

`\setlewis[<largeur de la lacune |>]{<distance atome déco>}{<longueur du trait>}{<code tikz>}`

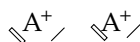
`\setlewis{4pt}{1.5em}{red}\lewis{26,B}`



`\setlewis[0.8ex]{}{}{line width=1pt}\lewis{2|,B}`



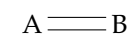
`\lewis{5|7,A^+} \Lewis[.1]{5|7,A^+}`



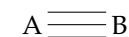
`\setlewisdist{1ex}\Lewis{1:3:5:7:,X}`



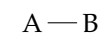
`\setdoublesep{1ex}\chemfig{A=B}`



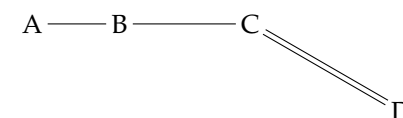
`\setdoublesep{1ex}\chemfig{A~B}`



`\setatomsep{2em}\chemfig{A-B}`



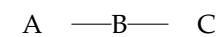
`\chemfig{A-B-[1.5]C=[:-30,2]D}`



`\setbondoffset{1em}\chemfig{A-B}`



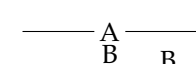
`\setbondoffset{1em}\chemfig{A-#(,Opt)B-#(Opt)C}`



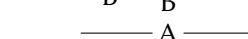
`\setcrambond{5mm}{2mm}{1mm}\chemfig{A>:B}`



`\chemfig{-\chembelow{A}{B}-}`



`\setstacksep{1ex}\chemfig{-\chemabove{A}{B}-}`



[<angle des liaisons>,<coefficient de longueur>,<numéro de l'atome de départ>,<numéro de l'atome d'arrivée>,<code tikz>]

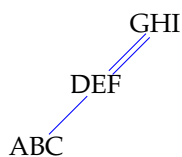
`\chemfig{A-[2,,,red,line width=2pt]B}`



`\chemfig{A-[,,,decorate,decoration=snake]B}`



`\chemfig{[1,,2,2,blue]ABC-DEF=GHI}`



7–Schémas réactionnels

Les schémas réactionnels doivent être placés entre `\schemestart` et `\schemestop`

Remarque : ne pas laisser de lignes blanches dans le code.

7.1–Les flèches

<code>A \arrow B</code>	$A \longrightarrow B$	<code>A \arrow{->} B</code>	$A \longrightarrow B$
<code>A \arrow{-/>} B</code>	$A \not\longrightarrow B$	<code>A \arrow{<-} B</code>	$A \longleftarrow B$
<code>A \arrow{<->} B</code>	$A \longleftrightarrow B$	<code>A \arrow{<=>} B</code>	$A \rightleftharpoons B$
<code>A \arrow{<->>} B</code>	$A \rightleftharpoons B$	<code>A \arrow{<<->} B</code>	$A \rightleftharpoons B$
<code>A \arrow{0} B</code>	$A \quad B$	<code>A \arrow{-U>[123][456]} B</code>	$A \xrightarrow[123]{456} B$

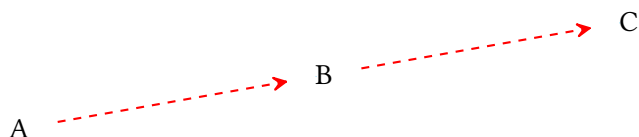
7.2–Modifications des flèches

`\setarrowdefault{angle,coeff,style}`

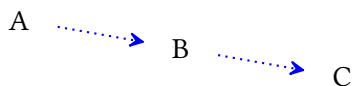
`\setarrowdefault{}` remet les options par défaut.

`\setarrowdefault{10,2,red,thick,dashed}`

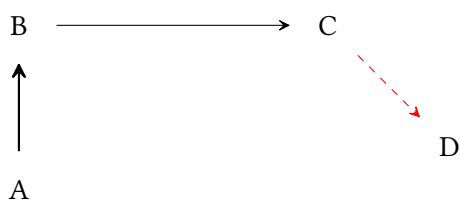
`\schemestart A\arrow B\arrow C\schemestop`



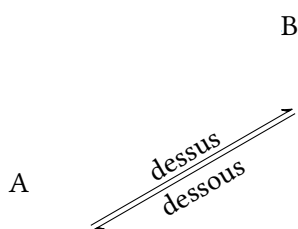
`\schemestart[-10,1,blue,dotted] A\arrow B\arrow C\schemestop`



`\schemestart A\arrow[90,,thick]B\arrow[,2]C \arrow[-45,,dashed,red]D \schemestop`



`\schemestart A\arrow{<=>[dessus][dessous][-1cm]}[30,2]B \schemestop`



`\schemestart`

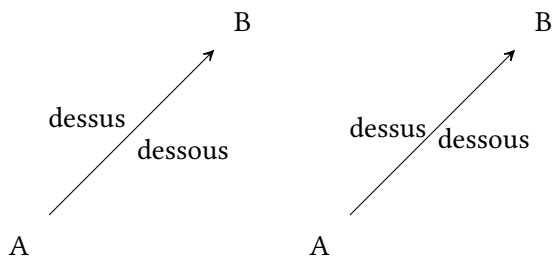
`A\arrow{->[*{0.south east}dessus][*{0.north west}dessous]}[45,2]B`

`\schemestop`

`\schemestart`

`A\arrow{->[*{0.0}dessus][*{0.180}dessous]}[45,2]B`

`\schemestop`



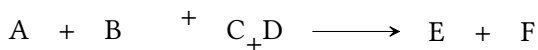
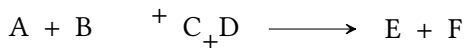
7.3–Le signe +

{<avant>, <après>, <décalage>}

On peut utiliser `\setandsign{<avant>, <après>, <décalage>}`

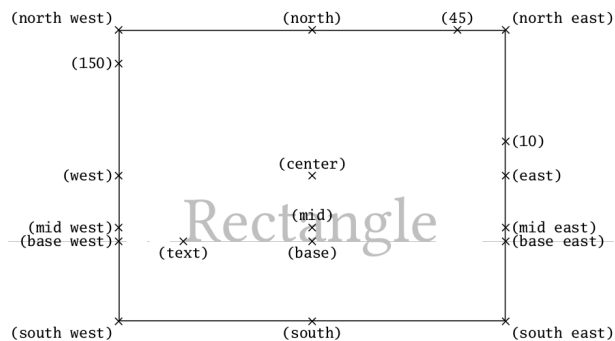
```
\schemestart
A\+B\+{2em, ,5pt}C\+{0pt,0pt,-5pt}D\arrow E\F
\schemestop
```

```
\setandsign{1em,1em,0pt}
\schemestart
A\+B\+{2em, ,5pt}C\+{0pt,0pt,-5pt}D\arrow E\F
\schemestop
```

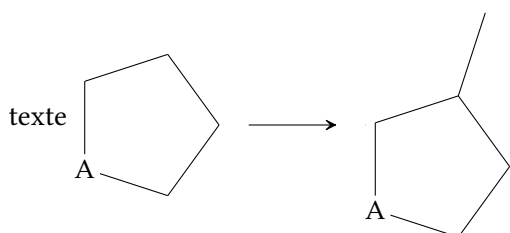


7.4–Positionnements et embranchements

Un schéma réactionnel est constitué de boites successives séparées par des flèches. Donc A + B forme une boite. Chaque boite possède des points de repérage qu'il est possible d'utiliser :



```
texte
\schemestart [] [west]
\chemfig{A*5(-----)}
\arrow(.east--.west)
\chemfig{A*5(---(-)--)}
\schemestop
```

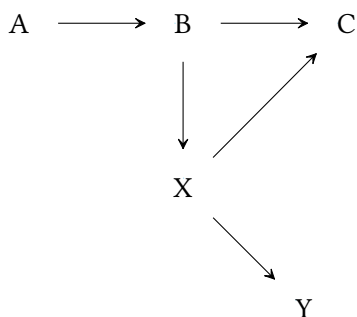


Les boites sont nommées par défaut successivement c1, c2...

```

\schemestart
A\arrow B\arrow C
\arrow{@c2--x}[-90]X\arrow[-45]Y
\arrow{@x--@c3}
\schemestop

```



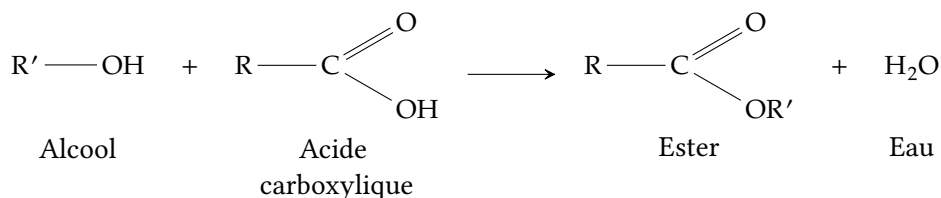
Remarque : une astuce pour scinder les boites A + B en plusieurs boites est d'utiliser la flèche invisible $\arrow{0}[,0]$

7.5-Placement des noms sous les formules

```

\schemestart
\chemnameinit{\chemfig{R-C(-[:30]OH)=[:30]O}}
\chemname{\chemfig{R'-OH}}{Alcool}
\+
\chemname{\chemfig{R-C(-[:30]OH)=[:30]O}}{Acide \carboxylique}
\arrow(.base east--.base west)
\chemname{\chemfig{R-C(-[:30]OR')=[:30]O}}{Ester}
\+
\chemname{\chemfig{H_2O}}{Eau}
\schemestop

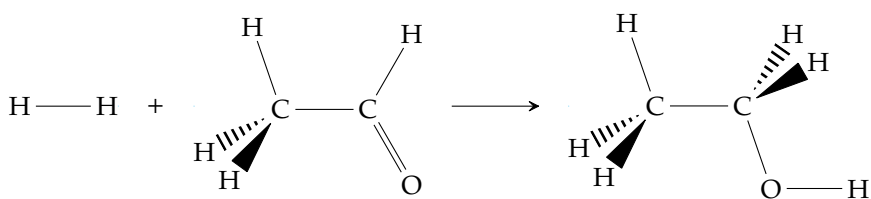
```



```

\schemestart
\chemfig{H-H}\arrow{0}[,0pt]\+\arrow{0}[,0pt]
\chemfig{[:71]H-C(<[:80]H)(<[:55]H)-[:71]C(-[:60]H)=[:60]O}
\arrow
\chemfig{[:71]H-C(<[:80]H)(<[:55]H)-[:71]C(<[:30]H)(<[:55]H)-[:71]O-[:71]H}
\schemestop
\chemmove{\node[below=2cm]at (c1) {dihydrogène}; }
\chemmove{\node[below=2cm]at (c3) {éthanal}; }
\chemmove{\node[below=2cm]at (c4) {éthanol}; }

```



dihydrogène

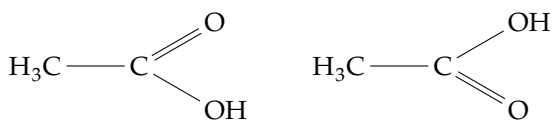
éthanal

éthanol

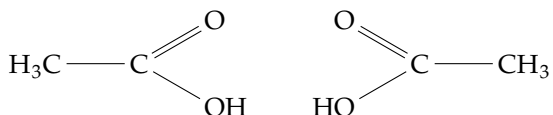
8-Divers

8.1-Molécules symétriques

```
\chemfig{H_3C-C(=[:30]O)-[: -30]OH}
\vflipnext\chemfig{H_3C-C(=[:30]O)-[: -30]OH}
```

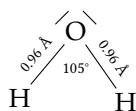


```
\chemfig{H_3C-C(=[:30]O)-[: -30]OH}
\hflipnext\chemfig{H_3C-C(=[:30]O)-[: -30]OH}
```



8.2-Affichage de la distance interatomique et des angles

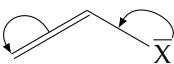
```
\chemfig{[:50]@{a}H-@{b}\lewis{13,0}-[: -105]@{c}H}
\chemmove{\path(a)--node[above,sloped]{\tiny 0.96~\AA}(b);}
\chemmove{\path(b)--node[above,sloped]{\tiny 0.96~\AA}(c);}
\chemmove{\node[below=3mm] at (b){\tiny 105°};}
```



9-Déplacements d'électrons

2 compilations successives sont nécessaires.

```
\chemfig{@{a}=_@{b}::30-@{c}::-60@{d}\lewis{2,X}}
\chemmove{\draw[-latex](b)..controls++(120:.5) and ++(120:.5)..(a);}
\chemmove{\draw[shorten <=3pt,-latex](d)..controls++(60:.5) and ++(60:.5)..(c);}
```



```
\chemfig{@{a}\lewis{1,X}}
\quad\quad
\chemfig{@{b}\lewis{2|,X}}
\chemmove[->,shorten <=3pt,shorten >=3pt]{
\draw(a.north east).. controls +(90:1cm) and +(90:1cm).. (b);}
```



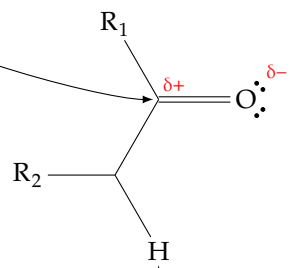
```
\hspace{3cm}\tikz[remember picture]\node(n1){\chemname{}{Attaques\nucléophiles}};
```

```
\hspace{5cm}\chemfig{R_2-(-[: -60]@{a}H)-[:60]@{b}(-[:120]R_1)(-[1,0.25,,,draw=none]\scriptstyle\color{red}\delta{-})
=lewis{1:7::,0}-[1,0.5,,,draw=none]\scriptstyle\color{red}\delta{-}}
```

```
\hspace{3cm}\chemname{}{Propriétés acides des atomes\tikz[remember picture]\node(n2){};
\\d'hydrogène en position $\alpha$}
```

```
\chemmove[-latex]{
\draw[shorten >=2pt](n1)..controls+(270:4em)and+(180:2em)..(b);
\draw[shorten >=2pt](n2)..controls+(0:2em)and+(270:2em)..(a);
}
```

Attaques
nucléophiles



Propriétés acides des atomes
d'hydrogène en position α