MYCHEMISTRY – EXAMPLES

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Create Reaction Schemes with LaTeX 2ε and Chemfig

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English documentation

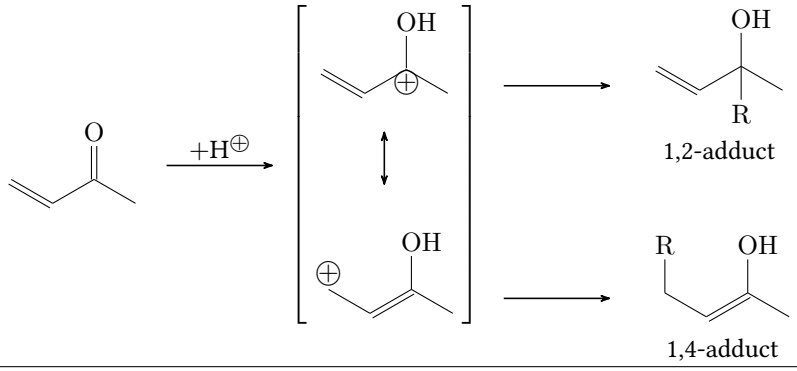
Since the documentation is already long enough I decided to provide an extra file containing only examples and a few words where to find possibly interesting code.
For all the undocumented little macros like \fscrp or \delm have a look in the chemmacros documentation.

Contents

1 Addition Reaction

A simple reaction scheme with two different products.

Reaction scheme 1 Addition Reaction

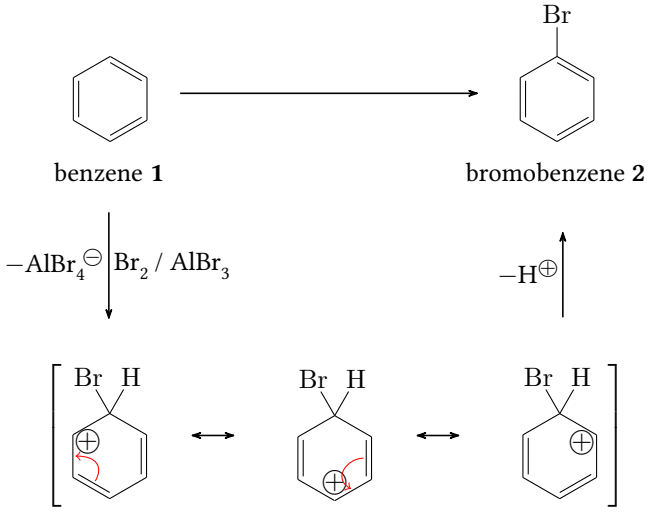



```
1  \begin{rxnscheme}[,]{Addition Reaction}
2   \reactant{ \chemfig{=_[::-30]-[::60](=[::60]O)-[::-60]} }
3   \arrow{ $+ \Hpl$ }{}
4   \mesomeric[,rf]{
5     \reactant{ \chemfig{=_[:-30]-[::60](-[::60]OH)
    (-[::-120,.3,,,white]\fplus)-[::-60]} }
6     \marrow[below]
7     \reactant[below]{ \chemfig{\fplus-[6,.3,,,white
    ]-[:-30]=_[::60](-[::60]OH)-[::-60]} }
8   }
9   \branch[right=of rf,,yshift=3em]{
10    \arrow{}{}
11    \reactant{ \chemname{\chemfig{=_[:-30]-[::60](-[::60]OH)
    (-[::-120]R)-[::-60]}}{1,2-adduct} }
12  }
13  \branch[right=of rf,,yshift=-5em]{
14    \arrow{}{}
15    \reactant{ \chemname{\chemfig{R
    -[6]-[:-30]=_[::60](-[::60]OH)-[::-60]}}{1,4-adduct} }
16  }
17 \end{rxnscheme}
```

2 Mesomerism

If you put something relative to an arrow you might have to consider that the arrow's anchor point is in the middle of the arrow. That's why `\mesomeric` is shifted with `yshift=-2.5em` in line 9.

Reaction scheme 2 Mesomerism



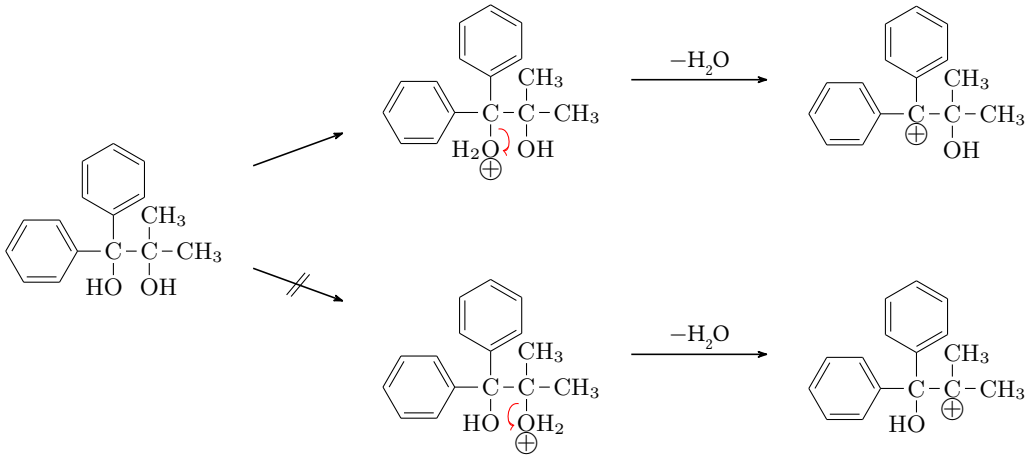

```
\begin{rxnscheme}[,,,.8]{Mesomerism}
 \setatomsep{1.6em}
 % main reaction:
 \reactant[,start]{ \chemname{\chemfig{*6(-=-=(-[,,,,white]\
 phantom{Br})-=)}}{benzene \cmpd{benzene}} }
 \arrow[,,2.8]{}{}
 \reactant{ \chemname{\chemfig{*6(-=-=(-Br)-=)}}{
 bromobenzene \cmpd{bromobenzene}} }
 % branch:
 \arrow[start.below,,,pfeil_a]{\ch{Br2} / \ch{AlBr3}}{$-\ch{
 AlBr4-}$}
 \mesomeric[!!pfeil_a.below!!,mesomerism,xshift=8.5em,!!
 yshift=-2.5em!!]{
   \reactant{
     \chemfig{*6(=[@{e1}]-=-(-[:120]Br)(-[:60]H)
 -(-[:-30,.4,,,white]\fplus)-[@{e2}])}
     \elmove{e1}{60:4mm}{e2}{0:4mm}
   }
   \marrow
   \reactant{
     \chemfig{*6(-(-[:90,.4,,,white]\fplus)-[@{e4}]=[@{e
 3}]-(-[:120]Br)(-[:60]H)-=)}
     \elmove{e3}{180:4mm}{e4}{150:4mm}
   }
   \marrow
   \reactant{
     \chemfig{*6(-=-(-[:-150,.4,,,white]\fplus)-(-[:120]Br)
 (-[:60]H)-=)}
   }
 }
 % last arrow inside a branch, since it cannot be shifted
 by itself:
```

```
    \branch[above=of mesomerism,,xshift=7.5em]{
      \arrow[above]{$-\Hpl$}{}
    }
  \end{rxnscheme}
```

3 The Former Titlepage

This scheme used to be on the title page of the examples file. It isn't any more but here's the scheme, anyway.

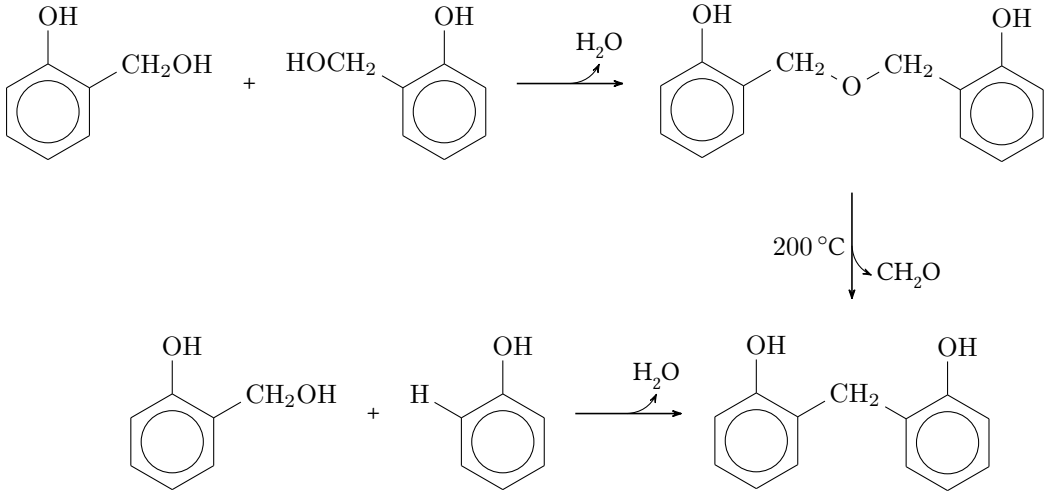
Reaction scheme 3 The Titlepage



```
\begin{rxn}[,.7]
 \setatomsep{1.5em}\footnotesize
 % reaction above:
 \reactant[,a]{ \chemfig{C(-[4]*6(=-=-=-))(-[2]*6(=-=-=-))
 (-[6,,,2]HO)-C(-[2]CH_3)(-[6]OH)-CH_3} }
 \arrow[a.45]{}{}
 \reactant[45]{ \chemfig{C(-[4]*6(=-=-=-))(-[2]*6(=-=-=-))
 (-[@{e1}6,,,2]H_2@{e2}\chembelow{O}{\fplus})-C(-[2]CH_3)
 (-[6]OH)-CH_3}\elmove{e1}{10:4mm}{e2}{-10:4mm} }
 \arrow[,,1.42]{$-\ch{H2O}$}{}
 \reactant{ \chemfig{\chembelow{C}{\fplus}(-[4]*6(=-=-=-))
 (-[2]*6(=-=-=-))-C(-[2]CH_3)(-[6]OH)-CH_3} }{}
 % going down:
 \arrow[a.-45,-|>]{}{}
 \reactant[-45]{ \chemfig{C(-[4]*6(=-=-=-))(-[2]*6(=-=-=-))
 (-[6,,,2]HO)-C(-[2]CH_3)(-[@{e3}6]@{e4}\chembelow{O}{\
 fplus}H_2)-CH_3}\elmove{e3}{170:4mm}{e4}{-170:4mm} }
 \arrow[,,1.42]{$-\ch{H2O}$}{}
 \reactant{ \chemfig{C(-[4]*6(=-=-=-))(-[2]*6(=-=-=-))
 (-[6,,,2]HO)-\chembelow{C}{\fplus}(-[2]CH_3)-CH_3} }
\end{rxn}
```

4 Condensation Reaction

Reaction scheme 4 Condensation Reaction

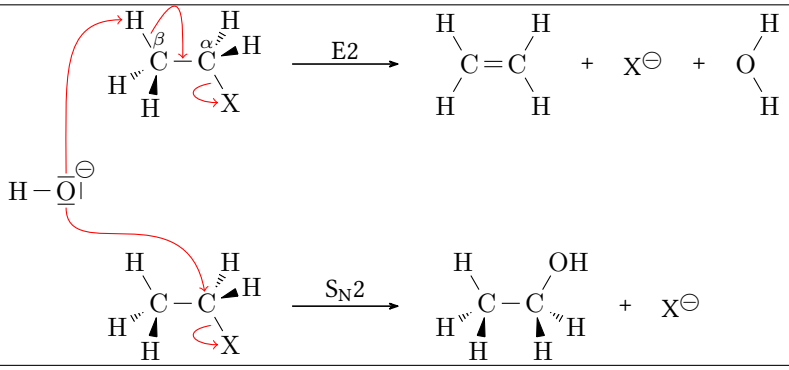



```
\begin{rxnscheme}{Condensation Reaction}
 \reactant{\chemfig{**6(---(-CH_2OH)-(-OH)--)}}
 \chemand
 \reactant{\chemfig{**6(----(-OH)-(-HOCH_2)-)}}
```

```
5    \arrow[,-+>]{}{\ch{H2O}}
6    \reactant{\chemfig{**6(---(-CH_2-[:-30]O-[:30]CH
     _2-[:-30]**6(-----(-OH)-))-(-OH)--)}}
7    \arrow[-90,-+>,,dec]{}{\ch{CH2O}}
8    \anywhere{dec.180,,xshift=-.2em}{\SI{200}{\celsius}}
9    \reactant[-90,target]{\chemfig{**6(---(-CH
     _2-[:-30]**6(-----(-OH)-))-(-OH)--)}}
10   \branch[left=of target]{
11     \reactant{\chemfig{**6(---(-CH_2OH)-(-OH)--)}}
12     \chemand
13     \reactant{\chemfig{**6(----(-OH)-(-H)-)}}
14     \arrow[,-+>]{}{\ch{H2O}}
15   }
16 \end{rxnscheme}
```

5 Substitution vs. Elimination

Reaction scheme 5 Substitution vs. Elimination



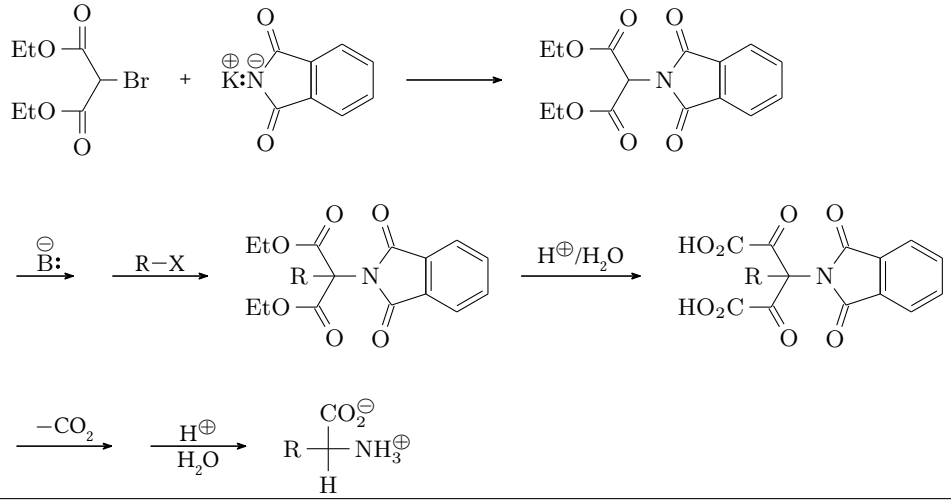
You may see in line 20 that the \elmove commands are put inside of \anywhere. This is necessary in order to produce the right scheme. But this time you can position \anywhere literally anywhere.

```
\begin{rxnscheme}{Substitution vs. Elimination}
 % first reaction:
 \reactant[,start_a]{\chemfig{@{H}H-[@{b1}:-60]\chemabove{C
 }{\scriptstyle\beta}(<[:-100]H)(<:[:-150]H)-[@{b2}]\
 chemabove{C}{\scriptstyle\alpha}(<[:20]H)(<:[:60]H)-[@{b
 3}:-60]@{X1}X}}
 \arrow{\mech[e2]{}
 \reactant{\chemfig{H-[:60]C(-[:120]H)=C(-[:60]H)-[:-60]H}}
 \chemand
 \reactant{\ch{X-}}
 \chemand
 \reactant{\chemfig{O(-[:60]H)-[:-60]H}}
 % second reaction:
 \reactant[start_a.-90,start_b,yshift=-4em]{\chemfig{H
 -[:-60]C(<[:-100]H)(<:[:-150]H)-@{C}C(<[:20]H)(<:[:60]H)-[
 @{b4}:-60]@{X2}X}}
 \arrow{\mech[2]}{}
 \reactant{\chemfig{H-[:-60]C(<[:-100]H)(<:[:-150]H)-C
 (<[:-80]H)(<:[:-30]H)-[:60]OH}}
 \chemand
 \reactant{\ch{X-}}
 % nucleophile/base:
 \anywhere{start_b.135,nuc,xshift=-3em,yshift=2em}{\chemfig{
 H-@{O}\chemabove{\lewis{026,O}}{\hspace{5mm}\fscrm}}}
 % electron movements:
 \anywhere{nuc.0}{
   \elmove{O}{90:1.5cm}{H}{180:1cm}
   \elmove{b1}{60:1cm}{b2}{90:5mm}
   \elmove{b3}{-170:5mm}{X1}{180:5mm}
   \elmove{O}{-90:1cm}{C}{100:1.5cm}
   \elmove{b4}{-170:5mm}{X2}{180:5mm}
 }
\end{rxnscheme}
```

6 Scheme with three Lines

```
\begin{rxnscheme}{Scheme with three Lines}
 \setatomsep{1.5em}
 \footnotesize
 \reactant[,start]{\chemfig{EtO-(=[2]O)-[:-60](-Br)
 -[:-120](=[6]O)-[4]EtO}}
 \chemand
 \reactant{\chemfig{*6(-=-=-*5(-(=O)-\chemabove{\lewis{4:,N
 }}{\fscrm}(-[4,.7,,,draw=none]\chemabove{K}{\fscrp})-(=O)
 --)=)}}
 \arrow{}{}
 \reactant{\chemfig{*6(-=-=-*5(-(=O)-N(-(-[::-60](=[::-60]O)
 -[::60]EtO)-[::60](=[::60]O)-[::-60]EtO)-(=O)--)=)}}
```

Reaction scheme 6 Scheme with three Lines



```
9   % newline, started with \anywhere:
10  \anywhere{start.-90,a,xshift=-4em,yshift=-5em}{}
11  \arrow[a.0,,.6]{\chemabove{\lewis{0:,B}}{\fscrm}}{}
12  \arrow{\ch{R-X}}{}
13  \reactant{\chemfig{*6(-=-=-*5(-(=O)-N(-(-[4]R)
    (-[::-60](=[::-60]O)-[::60]EtO)-[::60](=[::60]O)-[::-60]
    EtO)-(=O)--)=)}}
14  \arrow[,,1.25]{\Hpl/\ch{H2O}}{}
15  \reactant{\chemfig{*6(-=-=-*5(-(=O)-N(-(-[4]R)
    (-[::-60](=[::-60]O)-[::60]HO_2C)-[::60](=[::60]O)-[::-60]
    HO_2C)-(=O)--)=)}}
16  % newline, started with \anywhere:
17  \anywhere{a.-90,b,yshift=-7em}{}
18  \arrow[b.0]{$- {\ch{CO2}}$}{}
19  \arrow{\Hpl}{\ch{H2O}}
20  \reactant{\chemfig{R-(-[6]H)(-[2]C|O_2\mch)-NH_3\pch}}
21 \end{rxnscheme}
```

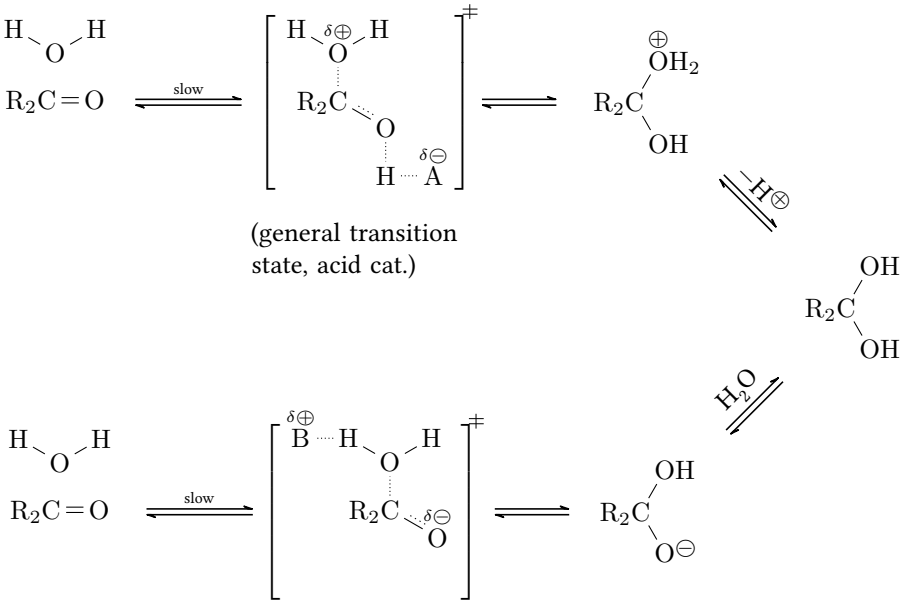
7 Hydratisation

A scheme with transition states.

For this example we first declare a style for the delocalized double bonds:

```
1  \pgfdeclaredecoration{ddbond}{initial}{%
2    \state{initial}[width=2pt]{%
3      \pgfpathlineto{\pgfpoint{2pt}{0pt}}%
4      \pgfpathmoveto{\pgfpoint{1.5pt}{2pt}}%
5      \pgfpathlineto{\pgfpoint{2pt}{2pt}}%
6      \pgfpathmoveto{\pgfpoint{2pt}{0pt}}%
7    }%
```

Reaction scheme 7 Hydratisation




```
    \state{final}{%
      \pgfpathlineto{\pgfpointdecoratedpathlast}%
    }%
  }%
  \tikzset{lddbond/.style={decorate,decoration=ddbond}}%
  \tikzset{rddbond/.style={decorate,decoration={ddbond,mirror
   }}}%
```

Now the delocalized double bond can be used via chemfig's fifth option (see the chemfig manual):

```
\chemfig{-[,,,,lddbond]-[,,,,rddbond]}
```

Then the whole code looks like follows:

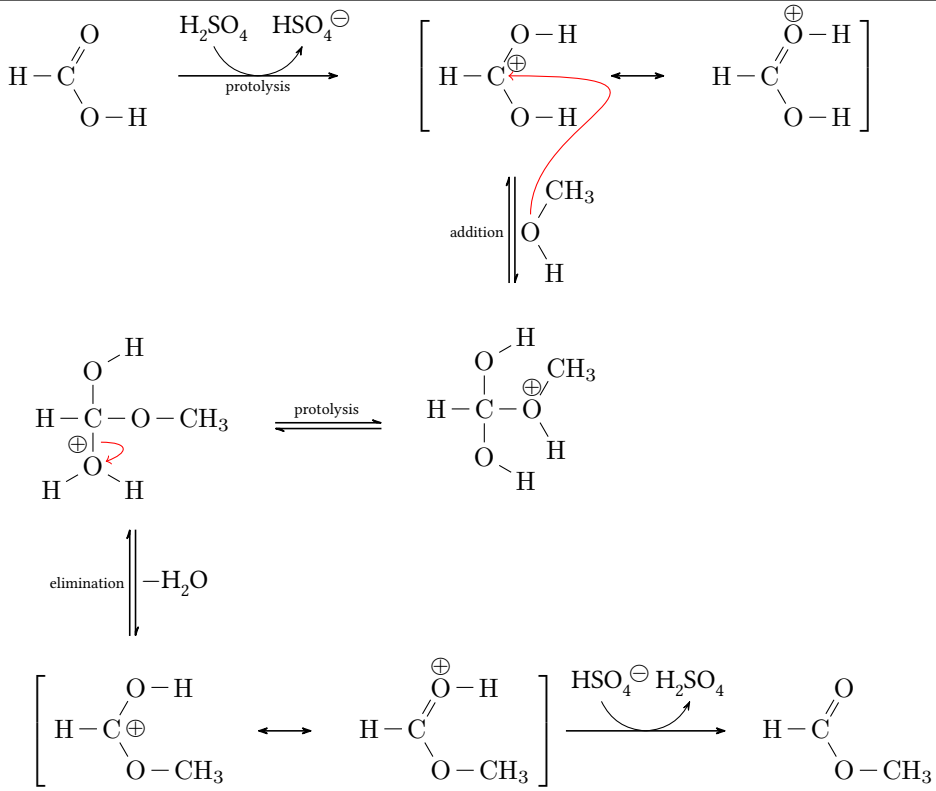
```
\begin{rxnscheme}{Hydratisation}
 \reactant[,carbonyl_A]{\chemfig{R_2C=O}}
 \anywhere{above=of carbonyl_A}{\chemfig{H-[:-30]O-[:30]H}}
 \arrow[,<=>]{\tiny slow}{}
 \transition[,transition_A]{\chemfig{R_2C(-[2,,2,,densely
 dotted]\chemabove{O}{\delp}(-[:150]H)-[:30]H)-[:-30,1.15,,,
 lddbond]O-[6,,,,densely dotted]H-[,,,,densely dotted]\
 chemabove{A}{\delm}}}
 \anywhere{below=of transition_A,,text width=3cm}{(general
 transition state, acid cat.)}
 \arrow[,<=>,.7]{}{}
 \reactant{\chemfig{R_2C(-[:60]\chemabove{O}{\fscrp}H_2)
 -[:-60]OH}}
 \arrow[below right,<=>,.7]{$-\Hpl$}{}
 \reactant[below right]{\chemfig{R_2C(-[:60]OH)-[:-60]OH}}
 \arrow[below left,<=>,.7]{}{\ch{H2O}}
 \reactant[below left,zw]{\chemfig{R_2C(-[:60]OH)-[:-60]O|\
 mch}}
 \arrow[left,<=>,.7]{}{}
 \transition[left,transition_B]{\chemfig{R_2C(-[2,,2,,
 densely dotted]O(-[:150]H-[4,,,,densely dotted]\chemabove{
 B}{\delp})-[:30]H)-[:-30,1.15,,,lddbond]\chemabove{O}{\
 delm}-[6,,,,draw=none]\phantom{H}}}
 \anywhere{below=of transition_B,,text width=3cm}{(general
 transition state, base cat.)}
 \arrow[left,<=>]{\tiny langsam}{}
 \reactant[left,carbonyl_B]{\chemfig{R_2C=O}}
 \anywhere{above=of carbonyl_B}{\chemfig{H-[:-30]O-[:30]H}}
\end{rxnscheme}
```

You can see that \anywhere was used several times, either to place molecules or to label molecules.

8 Esterification

```
\begin{rxn}{Esterification}
 \reactant{\chemfig{H-C(=[:60]O)-[:-60]O-H}}
 \arrow[,-+>,1.2,protolysis]{\ch{H2SO4}}{\ch{HSO4-}}
 \anywhere{below=of protolysis,,yshift=1em}{\tiny
 protolysis}
 \mesomeric{
   \reactant{\chemfig{H-@{a2}C(-[:60]O-H)(-[:30,.5,,,draw=
 none]{\fscrp})-[:-60]O-H}}
   \marrow
   \reactant{\chemfig{H-C(=[:60]\chemabove{O}{\fscrp}-H)
 -[:-60]O-H}}
 }
 \branch[below,,xshift=-5em]{
   \arrow[below,<=>]{\tiny addition}{\chemfig{H-[:120]@{a1}
```

Reaction scheme 8 Esterification

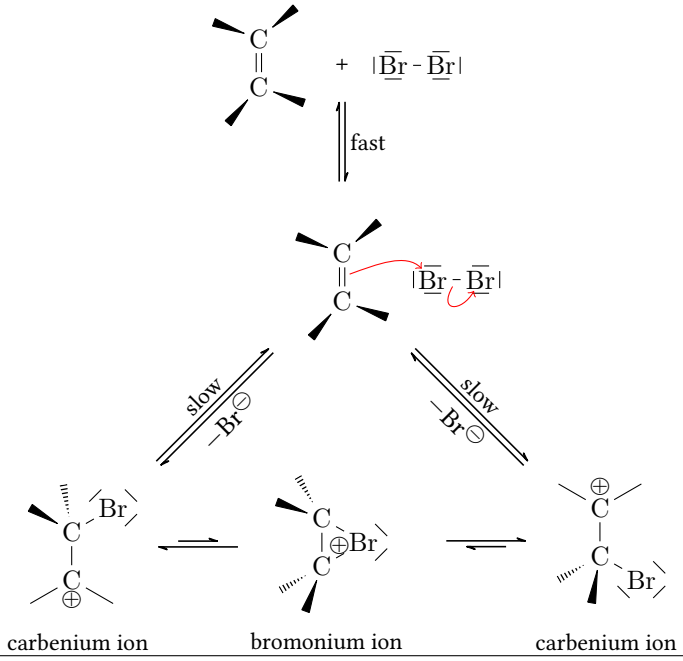


```
    O-[:60]CH_3}}
      \reactant[below]{
        \chemfig{H-C(-[2]O-[:30]H)(-\chemabove{O}{\fscrp
    }(-[:60]CH_3)-[:-60]H)-[6]O-[:-30]H}
        \elmove{a1}{90:1.5cm}{a2}{0:3cm}
      }
    }
    \branch[left,,yshift=-3.5em]{
      \arrow[left,<=>]{}{\tiny protolysis}
    }
    \reactant[left]{
      \chemfig{H-C(-[2]O-[:30]H)(-O-CH_3)-[@{b1}6]@{a3}\
    chemabove{O}{\hspace*{-4mm}\fscrp}(-[:-150]H)-[:-30]H}
      \elmove{b1}{0:5mm}{a3}{20:5mm}
    }
    \arrow[below,<=>]{$- {\ch{H2O}}$}{\tiny elimination}
    \mesomeric[below,,xshift=6em]{
      \reactant{\chemfig{H-C(-[:60]O-H)(-[,.5,,,draw=none]{\
    fscrp})-[:-60]O-CH_3}}
      \marrow
      \reactant{\chemfig{H-C(=[:60]\chemabove{O}{\fscrp}-H)
    -[:-60]O-CH_3}}
    }
    \arrow[,-+>,1.2]{\ch{HSO4-}}{\ch{H2SO4}}
    \reactant{\chemfig{H-C(=[:60]O)-[:-60]O-CH_3}}
  \end{rxnscheme}
```

9 Electrophilic Addition

This scheme forms a circle.

Reaction scheme 9 Electrophilic Addition



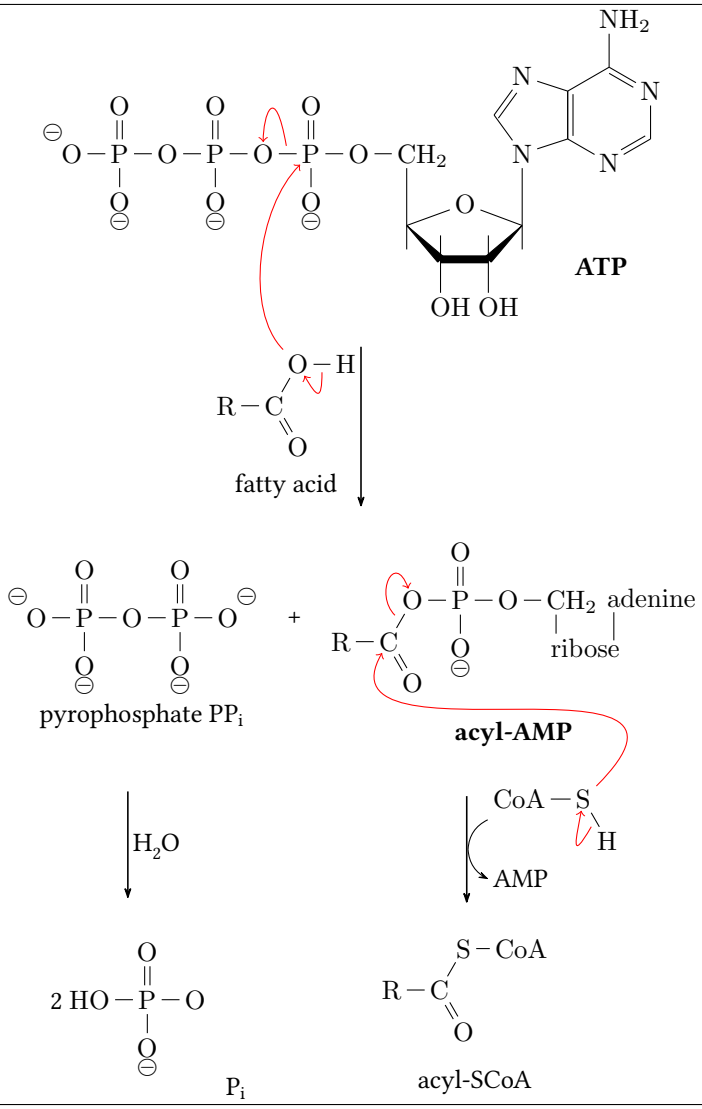

```
\begin{rxnscheme}{Electrophilic Addition}
 \setarrowlength{3em}
 \reactant{\chemfig{>[:-20]C(<[:40])=[6]C(<[:-130])<[:-20]}}

 \chemand[,plus]
 \reactant{\chemfig{\lewis{246,Br}-\lewis{026,Br}}}
 \arrow[plus.-90,<=>]{\footnotesize fast}{}
 \reactant[-90,attack]{\chemfig{>[:-20]C(<[:40])=[@{db}6]C
 (<[:-130])<[:-20]}}
 \anywhere{right=of attack}{
   \chemfig{@{Br1}\lewis{246,Br}-[@{b2}]@{Br2}\lewis{026,Br
 }}
   \elmove{db}{20:5mm}{Br1}{135:5mm}
   \elmove{b2}{-120:5mm}{Br2}{-120:5mm}
 }
 % to the left:
 \arrow[attack.-135,<=>,2]{$- {\ch{Br-}}$}{\footnotesize
 slow}
 \reactant[-135,carbenium_a]{\vflipnext\chemfig{-[:-30]\
 chembelow{C}{\fscrp}(-[:30])-[6]C(<[:-150])(<:[:-100])
 -[:-30]\lewis{137,Br}}}
 \anywhere{below=of carbenium_a}{\footnotesize carbenium
 ion}
 \arrow[,<<=>]{}{}
 \reactant[,bromonium]{\chemfig{>:[:-60]C?(<[:160])-[6]C
 (<[:-110])(<:[:-150])-[:30]\lewis{17,Br}?-[4,.5,,,draw=
 none]{\fscrp}}}
```

```
  \anywhere{below=of bromonium,,yshift=.35em}{\footnotesize
  bromonium ion}
  % to the right:
  \arrow[attack.-45,<=>,2]{\footnotesize slow}{$- {\ch{Br
  -}}$}
  \reactant[-45,carbenium_b]{\chemfig{-[:-30]\chemabove{C}{\
  fscrp}(-[:30])-[6]C(<:[:-150])(<[:-100])-[:-30]\lewis{157,
  Br}}}
  \anywhere{below=of carbenium_b}{\footnotesize carbenium
  ion}
  \arrow[left,<<=>]{}{}
  \mCsetup{reset}
\end{rxnscheme}
```

10 Activation of Fatty Acids

```
\begin{rxnscheme}{Activation of Fatty Acids}
 \reactant[,ATP]{\chemfig{\chemabove{O}{\hspace*{-5mm}\
 fscrm}-P(=[2]O)(-[6]\chembelow{O}{\fscrm})-O-P(=[2]O)(-[6]\
 chembelow{O}{\fscrm})-@{O1}O-[@{b1}]@{P}P(=[2]O)(-[6]\
 chembelow{O}{\fscrm})-O-CH_2-[6,1.5,1](-[6,.5])(-[:20,1.3]
 O?[a])<[7](-[2,.5])(-[6]OH)-[,,,,line width=3pt](-[2,.5])
 (-[6]OH)>[1]?[a](-[6,.5])-[2,1.5]N?[b]-[:18]([:30]*6(-N=-N
 =(-NH_2)-=))-[:90]-[:162]N=^[:-126]?[b]}}
 \anywhere{below right=of ATP,,xshift=-4em,yshift=3em}{\
 bfseries ATP}
 \arrow[below,,1.5]{\chemname{\chemfig{R-C(=[:-60]O)-[:60]@{
 O2}O-[@{b2}]H}}{fatty acid}}{}
 \branch[on chain=going below]{
   \reactant[,pyrophosphat]{
     \chemfig{\chemabove{O}{\hspace*{-5mm}\fscrm}-P(=[2]O)
 (-[6]\chembelow{O}{\fscrm})-O-P(=[2]O)(-[6]\chembelow{O}{\
 fscrm})-\chemabove{O}{\hspace*{5mm}\fscrm}}
     \elmove{b1}{100:1cm}{O1}{90:5mm}
     \elmove{O2}{135:1cm}{P}{-135:1cm}
     \elmove{b2}{-90:5mm}{O2}{-60:5mm}
     }
   \anywhere{below=of pyrophosphat}{pyrophosphate PP$_\text{
 i}$}
   \chemand
   \reactant[,acyl-amp]{\chemfig{R-@{C}C(=[:-60]O)-[@{b
 3}:60]@{O3}O-P(-[6]\chembelow{O}{\fscrm})(=[2]O)-O-CH
 _2-[6,,1,1]r|ibos|e-[2,1.05,3,1]A|denine}}
   \anywhere{below=of acyl-amp}{\bfseries acyl-AMP}
 }
 \branch[on chain=going below,,xshift=-8em]{
   \arrow[below]{\ch{H2O}}{}
   \reactant[below,Pi]{2~\chemfig{HO-P(=[2]O)(-[6]\
 chembelow{O}{\fscrm})-O}}
   \anywhere{below right=of Pi}{P$_\text{i}$}
```

Reaction scheme 10 Activation of Fatty Acids



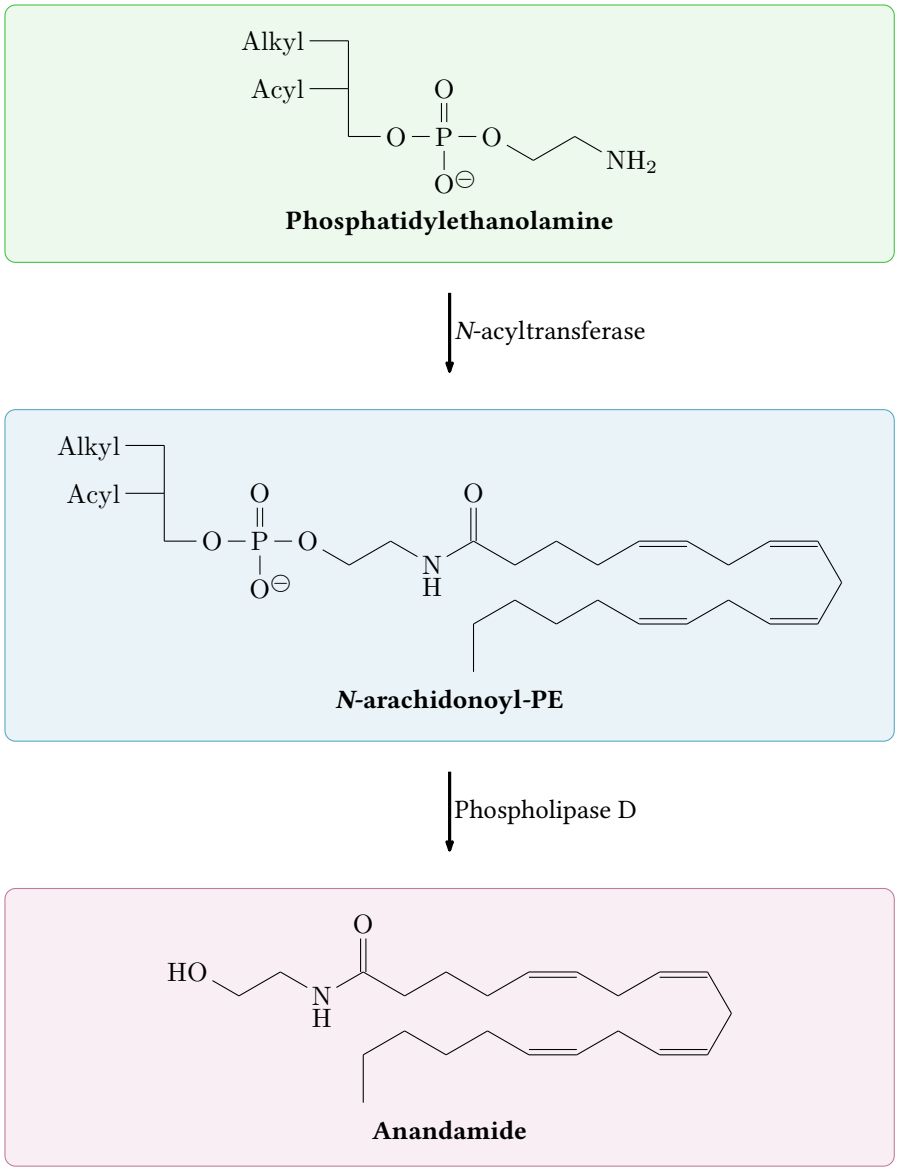
```
  }
  \branch[,,xshift=4em]{
    \arrow[below,-+>]{\chemfig{CoA-@{S}S-[@{b4}:-60]H}}{AMP}
    \reactant[below,acyl-SCoA]{
      \chemfig{R-C(=[:-60]O)-[:60]S-CoA}
      \elmove{S}{135:2cm}{C}{-135:1cm}
      \elmove{b3}{-45:5mm}{O3}{-70:7mm}
      \elmove{b4}{-120:7mm}{S}{-100:5mm}
    }
    \anywhere{below=of acyl-SCoA}{acyl-SCoA}
  }
\end{rxnscheme}
```

11 Change the layout with Ti*kZ*

This is an example for the usage of the <tikz> option. Please take a closer look at lines 5, 7, 11 and 15.

```
1  \begin{rxnscheme}{Change the layout with \TikZ}
2   \colorlet{mCgreen}{green!50!gray}
3   \colorlet{mCblue}{cyan!50!gray}
4   \colorlet{mCred}{magenta!50!gray}
5   !!\tikzset{reactant/.style={draw=#1,fill=#1!10,minimum
    width=.8\textwidth,inner sep=1em,rounded corners}}!!
6   \mCsetup{arrowlength=3em,arrowline=very thick}
7   \reactant[,,!!reactant=mCgreen!!]{
8     \chemname{\chemfig{Alky|l--[6](-[4,,,2]Acy|l)-[6]-O-P
    (=[2]O)(-[6]O|\mch)-O-[:-30]-[:30]-[:-30]NH_2}}{\bfseries
    Phosphatidylethanolamine}
9   }
10  \arrow[below]{}{\iupac{\N-acyl\|transferase}}
11  \reactant[below,,!!reactant=mCblue!!]{
12    \chemname{\chemfig{Alky|l--[6](-[4,,,2]Acy|l)-[6]-O-P
    (=[2]O)(-[6]O|\mch)-O-[:-30]-[:30]-[:-30]\chembelow{N}{H
    }-[:30](=[2]O)
    -[:-30]-[:30]-[:-30]-[:30]=_-[:-30]-[:30]=_-[:-60]
    -[::-60]=_[:180]-[::-30]-[::60]=_[:180]-[::-30]-
    [::60]-[::-60]-[::60]-[6]}}{\bfseries\iupac{\N\-
    arachidonoyl\-PE}}
13  }
14  \arrow[below]{}{Phospholipase D}
15  \reactant[below,,!!reactant=mCred!!]{
16    \chemname{\chemfig{HO-[:-30]-[:30]-[:-30]\chembelow{N}{H
    }-[:30](=[2]O)
    -[:-30]-[:30]-[:-30]-[:30]=_-[:-30]-[:30]=_-[:-60]
    -[::-60]=_[:180]-[::-30]-[::60]=_[:180]-[::-30]-
    [::60]-[::-60]-[::60]-[6]}}{\bfseries Anandamide}
17  }
```

Reaction scheme 11 Change the layout with Ti*k*Z

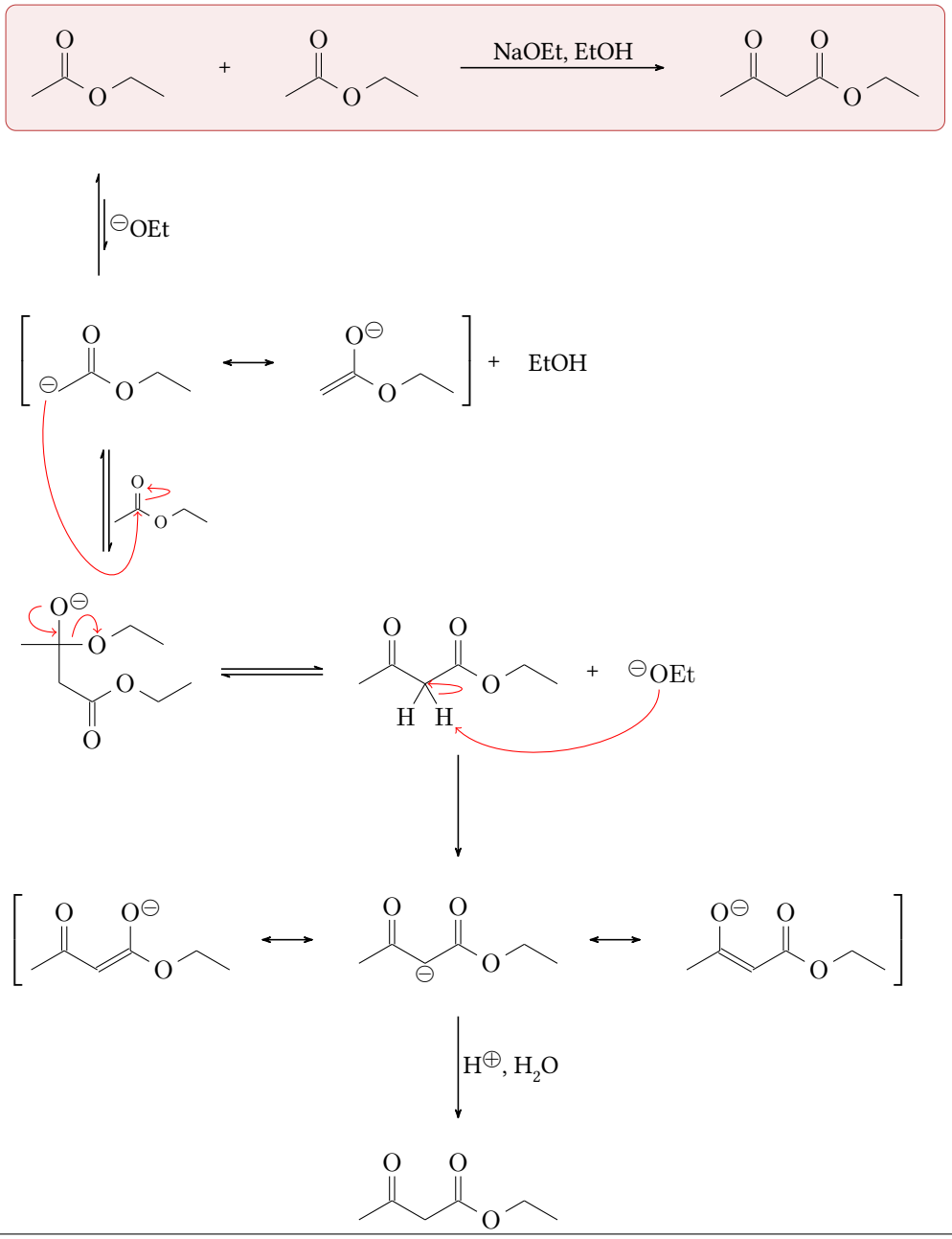


```
  \mCsetup{reset}
\end{rxnscheme}
```

12 Claisen-Kondensation

```
\begin{rxnscheme}{Claisen-Kondensation}
 \colorlet{mCred}{red!50!gray}
 \setatomsep{1.5em}
 % Ergebnis:
 \branch[,one,draw=mCred,fill=mCred!10,rounded corners,
 inner sep=.5em]{
   \reactant{\chemfig{[:30]-(=[2]O)-[:-30]O--[:-30]}}
   \chemand
   \reactant{\chemfig{[:30]-(=[2]O)-[:-30]O--[:-30]}}
   \arrow[,,2]{\ch{NaOEt}, \ch{EtOH}}{}
   \reactant{\chemfig{[:30]-(=[2]O)-[:-30]-(=[2]O)-[:-30]O
 --[:-30]}}
 }
 % Mechanismus:
 \branch[-90,,xshift=-13.5em]{
   \arrow[-90,<=>]{\ch{^-OEt}}{}
 }
 \mesomeric[-90,two,xshift=4.5em]{
   \reactant{\chemfig{[:30](-[:150,.3,,,draw=none]@{C1}\
 fscrm)-(=[2]O)-[:-30]O--[:-30]}}
   \marrow
   \reactant{\chemfig{[:30]=(-[2]O|\mch)-[:-30]O--[:-30]}}
 }
 \chemand
 \reactant{\ch{EtOH}}
 \branch[two.-90,three,xshift=-5.5em]{
   \arrow[-90,<=>,,,both]{\chemfig[][scale=.7]{[:30]-@{C
 2}(=[@{b1}2]O@{O1})-[:-30]O--[:-30]}}{}
 }
 \reactant[three.-90]{\chemfig{-(-[@{b2}2]@{O2}O|\mch)
 (-[6]-[:-30](=[6]O)-[:30]O-[:-30]-[:30])-[@{b3}]@{O3}O
 -[:30]-[:-30]}}
 \arrow[,<=>]{}{}
 \reactant[,four]{\chemfig{[:30]-(=[2]O)-[:-30]@{C
 3}(-[:-120]H)(-[@{b4}:-60]H@{H})-(=[2]O)-[:-30]O--[:-30]}}
 \chemand
 \reactant{\chemfig{\mch @{O4}OEt}}
 \arrow[four.-90]{}{}
 \mesomeric[-90]{
   \reactant{\chemfig{[:30]-(=[2]O)-[:-30]=(-[2]O|\mch)
 -[:-30]O--[:-30]}}
   \marrow
   \reactant{\chemfig{[:30]-(=[2]O)-[:-30](-[6,.3,,,draw=
 none]\fscrm)-(=[2]O)-[:-30]O--[:-30]}}
   \marrow
```

Reaction scheme 12 Claisen-Kondensation



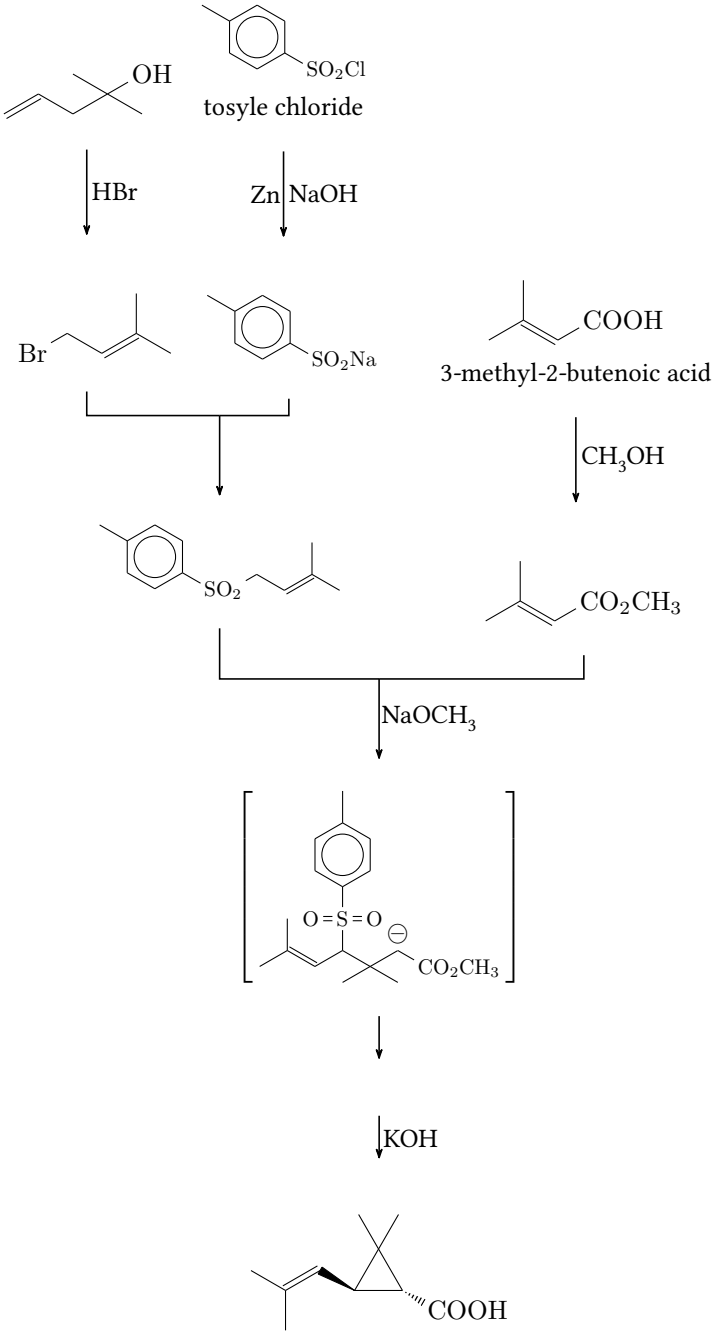
```
    \reactant{\chemfig{[:30]-(-[2]O|\mch)=[:-30]-(=[2]O)
  -[:-30]O--[:-30]}}
  }
  \arrow[-90]{\Hpl, \ch{H2O}}{}
  \reactant[-90]{\chemfig{[:30]-(=[2]O)-[:-30]-(=[2]O)
  -[:-30]O--[:-30]}}
  \anywhere{one.0}{
    \elmove{C1}{-100:2cm}{C2}{-90:2cm}
    \elmove{b1}{10:5mm}{O1}{0:5mm}
    \elmove{O2}{180:5mm}{b2}{180:5mm}
    \elmove{b3}{80:5mm}{O3}{90:5mm}
    \elmove{b4}{0:5mm}{C3}{0:7mm}
    \elmove{O4}{-90:1cm}{H}{-45:1cm}
  }
\end{rxnscheme}
```

13 Extensive Synthesis

As last example we can create extensive syntheses, using the \merge command.

```
\begin{rxnscheme}[,,,.8]{Extensive Synthesis}
 \setatomsep{1.5em}
 \branch[,start_left]{
   \reactant{\chemfig{=_[::30]-[::-60]-[::60](-[::-60])
 (-[::120])-[::0]OH}}
   \arrow[below]{\ch{HBr}}{}
   \reactant[below]{\chemfig{Br
 -[::30]-[::-60]=_[::60](-[::-60])-[::60]}}
 }
 \branch[right=of start_left,start_center,yshift=1em]{
   \reactant{\chemname{\chemfig[][scale=.8]{**6(--(-SO_2Cl)
 ---(-)-)}}{tosyle chloride}}
   \arrow[below]{\ch{NaOH}}{\ch{Zn}}
   \reactant[below]{\chemfig[][scale=.8]{**6(--(-SO_2Na)
 ---(-)-)}}
 }
 \branch[right=of start_center,start_right,xshift=3em,
 yshift=-10em]{
   \reactant{\chemname{\chemfig{-[::30](-[::60])
 =_[::-60]-[::60]COOH}}{\iupac{3\-methyl\-2\-butenoic acid
 }}}
   \arrow[below]{\ch{CH3OH}}{}
   \reactant[below]{\chemfig{-[::30](-[::60])
 =_[::-60]-[::60]CO_2CH_3}}
 }
 \branch[below=of start_left,target_one,xshift=5em,yshift
 =-5em]{
   \reactant{\chemfig[][scale=.8]{**6(--(-SO
 _2-[:30]-[::-60]=_[::60](-[::60])-[::-60])---(-)-)}}
 }
```

Reaction scheme 13 Extensive Synthesis



trans-chrysanthemum acid

```
21    \branch[below=of target_one,target_two,xshift=6em,yshift
      =-6em]{
22      \mesomeric{\chemfig[][scale=.8]{-[::30](-[::60])
      =^[::-60]-[::60](-[::60]S(=[::90]O)(=[::-90]O)
      -[::0]**6(---(-)---))-[::-60](-[::0])(-[::-120])
      -[::60](-[::60,.5,,,white]\fminus)-[::-60]CO_2CH_3}}
23      \arrow[below,,.5]{}{}
24      \arrow[below,,.5]{\ch{KOH}}{}
25      \reactant[below]{\chemname{\chemfig{-[::-30](-[::-60])
      =^[::60]>[::-60](-[::90,1.2])
      -[::30,1.2](-[::120,1.2](-[::-60])-[::0])<:[::-30]COOH}}{\
      iupac{\trans\-chrysanthemum acid}}
26    }
27    \merge{target_one}{start_left}{start_center}
28    \merge[\ch{NaOCH3}]{target_two}{target_one}{start_right}
29  \end{rxnscheme}
```