myChemistry

v1.5.1

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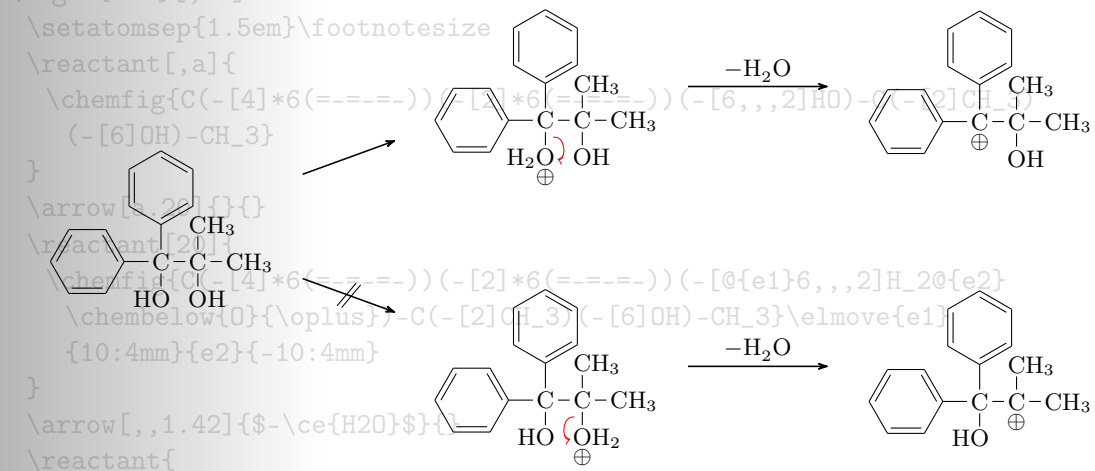
Examples




```
\begin{rxn}[,.7]
 \setatomsep{1.5em}\footnotesize
 \reactant[,a]{
  \chemfig{C(-[4]*6(=-=-=-))(-[2]*6(=-=-=-))(-[6,,,2]HO)-C(-[2]CH_3)
   (-[6]OH)-CH_3}
 }
 \arrow[a.2cm]{}{}
 \reactant[2]{
  \chemfig{C(-[4]*6(=-=-=-))(-[2]*6(=-=-=-))(-[@{e1}6,,,2]H_2@{e2}
   \chembelow{O}{\oplus}}-C(-[2]CH_3)(-[6]OH)-CH_3}\elmove{e1}
   {10:4mm}{e2}{-10:4mm}
 }
 \arrow[,,1.42]{$-\ce{H2O}$}{}
 \reactant{
  \chemfig{\chembelow{C}{\oplus}(-[4]*6(=-=-=-))(-[2]
  *6(=-=-=-))-C(-[2]CH_3)(-[6]OH)-CH_3}
 }
 \arrow[a.-20,-|>]{}{}
 \reactant[-20]{
  \chemfig{C(-[4]*6(=-=-=-))(-[2]*6(=-=-=-))(-[6,,,2]HO)-C(-[2]CH_3)
   (-[@{e3}6]@{e4}\chembelow{O}{\oplus}H_2)-CH_3}\elmove{e3}
   {170:4mm}{e4}{-170:4mm}
 }
 \arrow[,,1.42]{$-\ce{H2O}$}{}
 \reactant{
  \chemfig{C(-[4]*6(=-=-=-))(-[2]*6(=-=-=-))(-[6,,,2]HO)-
   \chembelow{C}{\oplus}(-[2]CH_3)-CH_3}
 }
\end{rxn}
```

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.

Example Schemes

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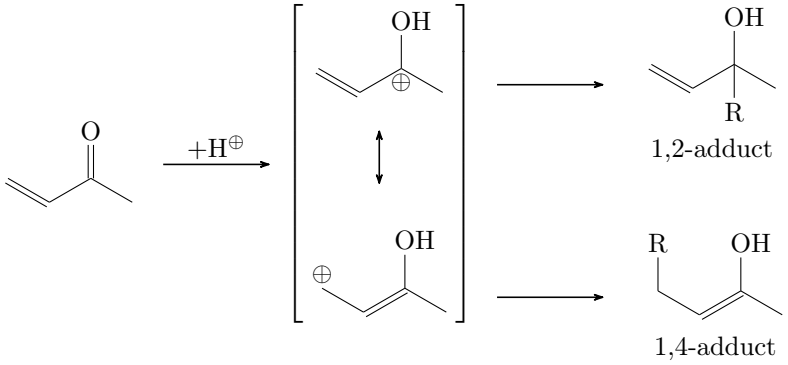
1 Addition Reaction

A simple reaction scheme with two different products.

Reaction scheme 1 Addition Reaction

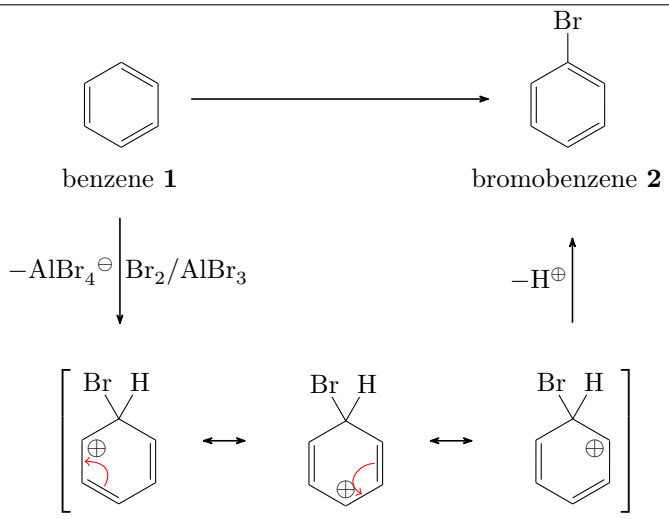



```
\begin{rxnscheme}[,H]{Addition Reaction}
 \reactant{ \chemfig{=_[::-30]-[::60](=[::60]O)-[::-60]}
    }
 \arrow{ $+ \Hpl$ }{}
 \mesomeric[,rf]{
   \reactant{ \chemfig{=_[:-30]-[::60](-[::60]OH)
      (-[::-120,.3,,,white]\oplus)-[::-60]} }
   \marrow[below]
   \reactant[below]{ \chemfig{\oplus-[6,.3,,,white
      ]-[:-30]=_[::60](-[::60]OH)-[::-60]} }
 }
```

```
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

Reaction scheme 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.

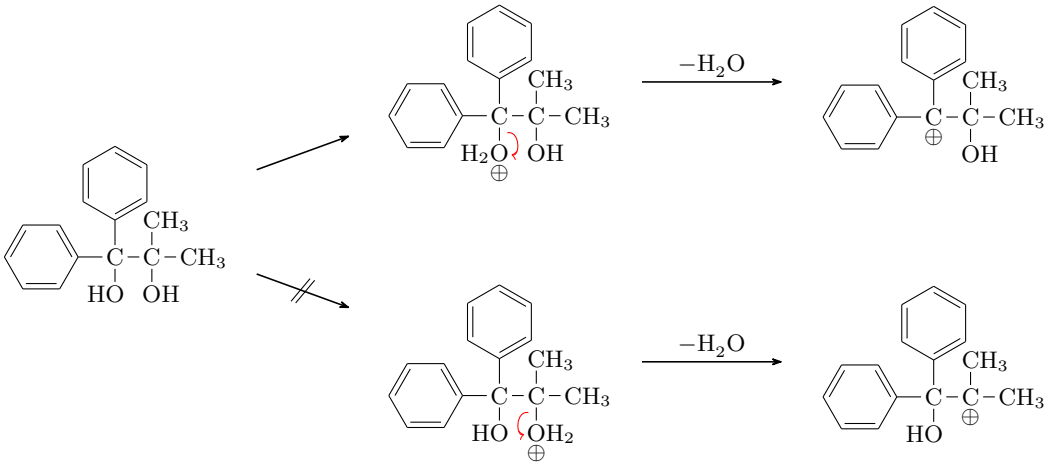
```
1   \begin{rxnscheme}[,H,,.8]{Mesomerism}
2    \setatomsep{1.6em}
3    % main reaction:
4    \reactant[,start]{ \chemname{\chemfig{*6(-=-=(-[,,,,
        white]\phantom{Br})-=)}}{benzene \compound{benzene}}
        }
5    \arrow[,,2.8]{}{}
```

```
    \reactant{ \chemname{\chemfig{*6(-=-=(-Br)-=)}}{
       bromobenzene \compound{bromobenzene}} }
    % branch:
    \arrow[start.below,,,pfeil_a]{\ce{Br2 / AlBr3}}{$-\ce{
       AlBr4\om}$}
    \mesomeric[pfeil_a.below,mesomerism,xshift=8.5em,yshift
       =-2.5em]{
      \reactant{
        \chemfig{*6(=[@{e1}]-=-(-[:120]Br)(-[:60]H)
           -(-[:-30,.4,,,white]\oplus)-[@{e2}])}
        \elmove{e1}{60:4mm}{e2}{0:4mm}
      }
      \marrow
      \reactant{
        \chemfig{*6(-(-[:90,.4,,,white]\oplus)-[@{e4}]=[@{e
           3}]-(-[:120]Br)(-[:60]H)-=)}
        \elmove{e3}{180:4mm}{e4}{150:4mm}
      }
      \marrow
      \reactant{
        \chemfig{*6(-=-(-[:-150,.4,,,white]\oplus)-(-[: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 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}{\oplus})-C(-[2]
      CH_3)(-[6]OH)-CH_3}\elmove{e1}{10:4mm}{e2}{-10:4mm} }
   \arrow[,,1.42]{$-\ce{H2O}$}{}
```

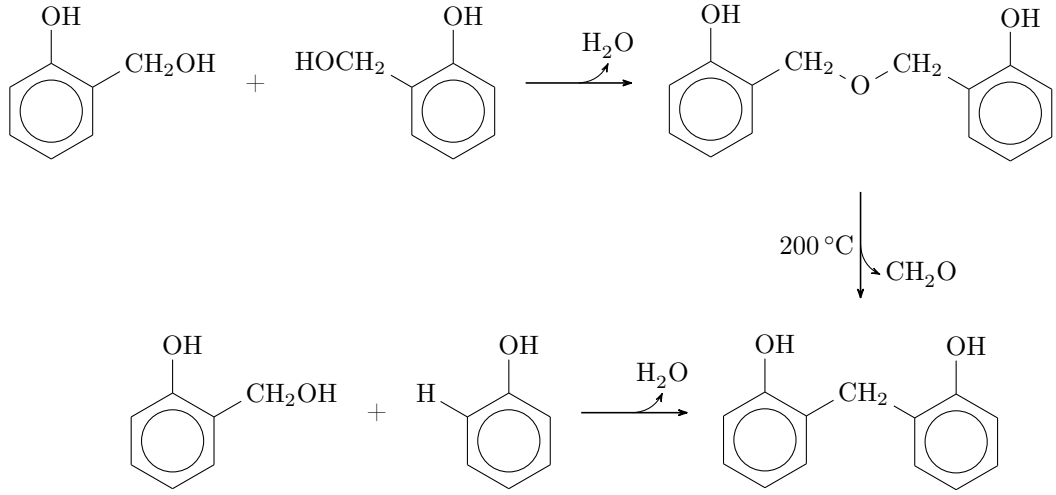
Reaction scheme 3 The Titlepage



```
8   \reactant{ \chemfig{\chembelow{C}{\oplus}(-[4]*6(=-=-=-)
       )(-[2]*6(=-=-=-))-C(-[2]CH_3)(-[6]OH)-CH_3} }{}
9   % going down:
10  \arrow[a.-45,-|>]{}{}
11  \reactant[-45]{ \chemfig{C(-[4]*6(=-=-=-))
       (-[2]*6(=-=-=-))(-[6,,,2]HO)-C(-[2]CH_3)(-[@{e3}6]@{e
       4}\chembelow{O}{\oplus}H_2)-CH_3}\elmove{e3}{170:4mm
       }{e4}{-170:4mm} }
12  \arrow[,,1.42]{$-\ce{H2O}$}{}
13  \reactant{ \chemfig{C(-[4]*6(=-=-=-))(-[2]*6(=-=-=-))
       (-[6,,,2]HO)-\chembelow{C}{\oplus}(-[2]CH_3)-CH_3} }
14  \end{rxn}
```

4 Condensation Reaction

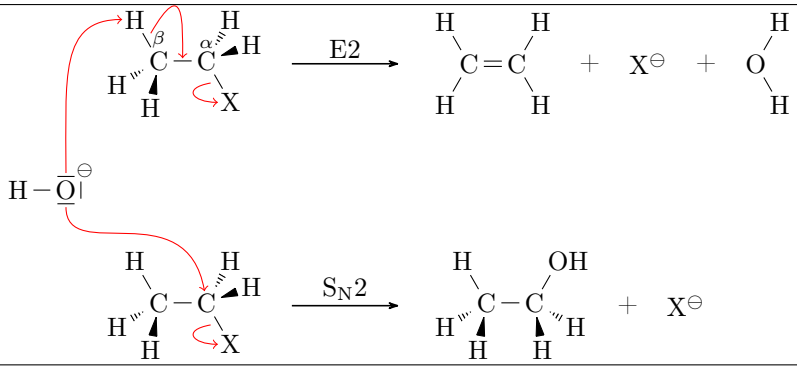
Reaction scheme 4 Condensation Reaction




```
\begin{rxnscheme}[,H]{Condensation Reaction}
 \reactant{\chemfig{**6(---(-CH_2OH)-(-OH)--)}}
 \chemand
 \reactant{\chemfig{**6(----(-OH)-(-HOCH_2)-)}}
 \arrow[,-+>]{}{\ce{H2O}}
 \reactant{\chemfig{**6(---(-CH_2-[:-30]O-[:30]CH
    _2-[:-30]**6(-----(-OH)-))-(-OH)--)}}
 \arrow[-90,-+>,,dec]{}{\ce{CH2O}}
 \anywhere{dec.180,,xshift=-.2em}{\SI{200}{\celsius}}
 \reactant[-90,target]{\chemfig{**6(---(-CH
    _2-[:-30]**6(-----(-OH)-))-(-OH)--)}}
 \branch[left=of target]{
   \reactant{\chemfig{**6(---(-CH_2OH)-(-OH)--)}}
   \chemand
   \reactant{\chemfig{**6(----(-OH)-(-H)-)}}
   \arrow[,-+>]{}{\ce{H2O}}
 }
\end{rxnscheme}
```

5 Substitution vs. Elimination

Reaction scheme 5 Substitution vs. Elimination



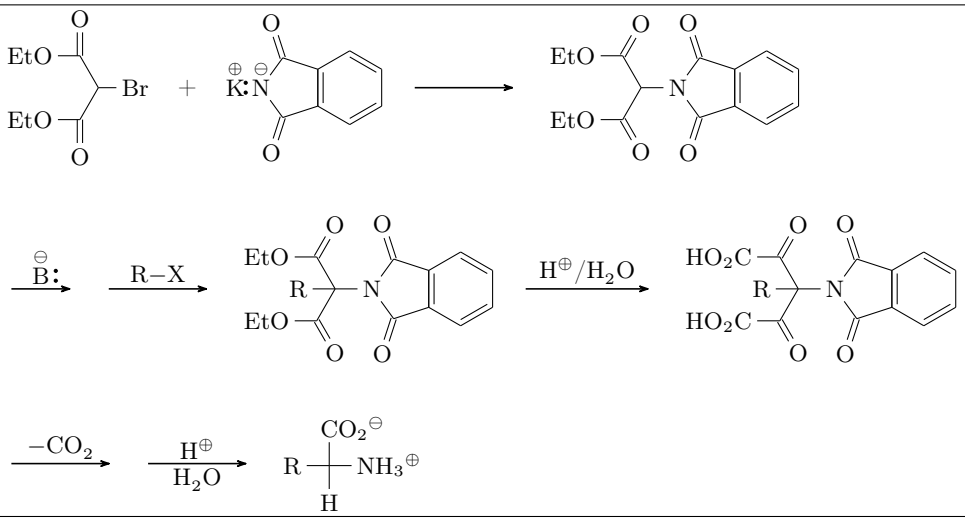
You may see in line 20 that the \elmove commands are put inside of \anywhere. This is necessary in order to produce the right scheme. But this time you can position \anywhere literally anywhere.

```
1  \newcommand*\scrom{\scriptstyle\ominus}
2  \begin{rxnscheme}[,H]{Substitution vs. Elimination}
3   % first reaction:
4   \reactant[,start_a]{\chemfig{@{H}H-[@{b1}:-60]\chemabove
       {C}{\scriptstyle\beta}(<[:-100]H)(<:[:-150]H)-[@{b
       2}]\chemabove{C}{\scriptstyle\alpha}(<[:20]H)(<:[:60]
       H)-[@{b3}:-60]@{X1}X}}
5   \arrow{E2}{}
6   \reactant{\chemfig{H-[:60]C(-[:120]H)=C(-[:60]H)-[:-60]H
       }}
7   \chemand
8   \reactant{\ce{X\om}}
9   \chemand
10  \reactant{\chemfig{O(-[:60]H)-[:-60]H}}
11  % second reaction:
12  \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}}
13  \arrow{S$_\text{N}$2}{}
14  \reactant{\chemfig{H-[:-60]C(<[:-100]H)(<:[:-150]H)-C
       (<[:-80]H)(<:[:-30]H)-[:60]OH}}
15  \chemand
16  \reactant{\ce{X\om}}
17  % nucleophile/base:
18  \anywhere{start_b.135,nuc,xshift=-3em,yshift=2em}{\
       chemfig{H-@{O}\chemabove{\lewis{026,O}}{\hspace{5mm}\
```

```
      scrom}}}
    % 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

Reaction scheme 6 Scheme with three Lines




```
  \newcommand*\scrom{\scriptstyle\ominus}
  \newcommand*\scrop{\scriptstyle\oplus}
  \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}}{\scrom}(-[4,.7,,,draw=none]\chemabove{K}{\
      scrop})-(=O)--)=)}}
   \arrow{}{}
```

```
    \reactant{\chemfig{*6(-=-=-*5(-(=O)-N
       (-(-[::-60](=[::-60]O)-[::60]EtO)-[::60](=[::60]O)
       -[::-60]EtO)-(=O)--)=)}}
    % newline, started with \anywhere:
    \anywhere{start.-90,a,xshift=-4em,yshift=-5em}{}
    \arrow[a.0,,.6]{\chemabove{\lewis{0:,B}}{\scrom}}{}
    \arrow{\ce{R-X}}{}
    \reactant{\chemfig{*6(-=-=-*5(-(=O)-N(-(-[4]R)
       (-[::-60](=[::-60]O)-[::60]EtO)-[::60](=[::60]O)
       -[::-60]EtO)-(=O)--)=)}}
    \arrow[,,1.25]{\Hpl/\ce{H2O}}{}
    \reactant{\chemfig{*6(-=-=-*5(-(=O)-N(-(-[4]R)
       (-[::-60](=[::-60]O)-[::60]HO_2C)-[::60](=[::60]O)
       -[::-60]HO_2C)-(=O)--)=)}}
    % newline, started with \anywhere:
    \anywhere{a.-90,b,yshift=-7em}{}
    \arrow[b.0]{\ce{- CO2}}{}
    \arrow{\Hpl}{\ce{H2O}}
    \reactant{\chemfig{R-(-[6]H)(-[2]C|O_2\om)-NH_3\op}}
  \end{rxnscheme}
```

7 Hydratisation

A scheme with transition states.

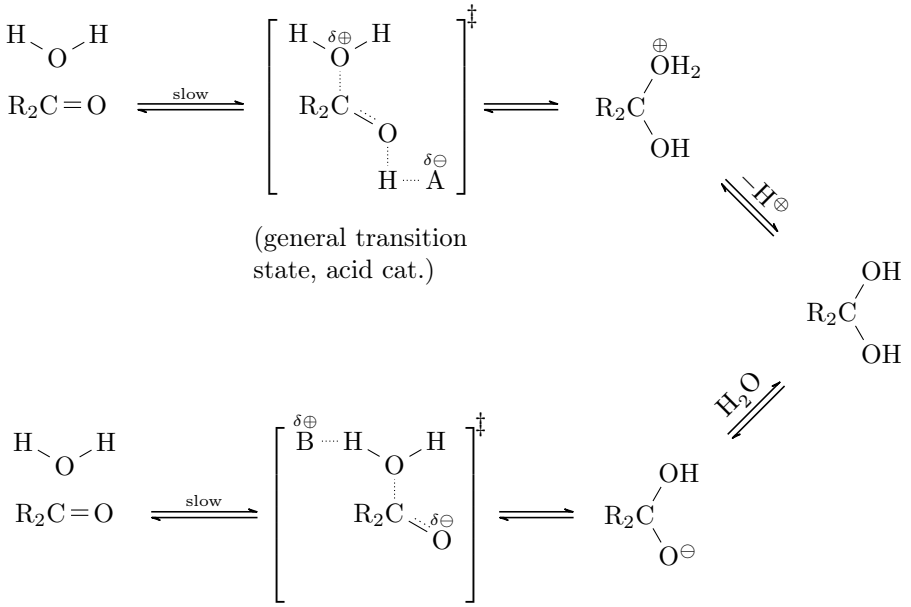
For this example we first declare a style for the delocalized double bonds:

```
\pgfdeclaredecoration{ddbond}{initial}{%
  \state{initial}[width=2pt]{%
    \pgfpathlineto{\pgfpoint{2pt}{0pt}}%
    \pgfpathmoveto{\pgfpoint{1.5pt}{2pt}}%
    \pgfpathlineto{\pgfpoint{2pt}{2pt}}%
    \pgfpathmoveto{\pgfpoint{2pt}{0pt}}%
  }%
  \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]}
```

Reaction scheme 7 Hydratisation



Further we define the two commands

```
\newcommand*\delm{\ensuremath{\text{\tiny$\delta\ominus$}}}%
\newcommand*\delp{\ensuremath{\text{\tiny$\delta\oplus$}}}%
```

to use the partial charges without effort.

Then the whole code looks like follows:

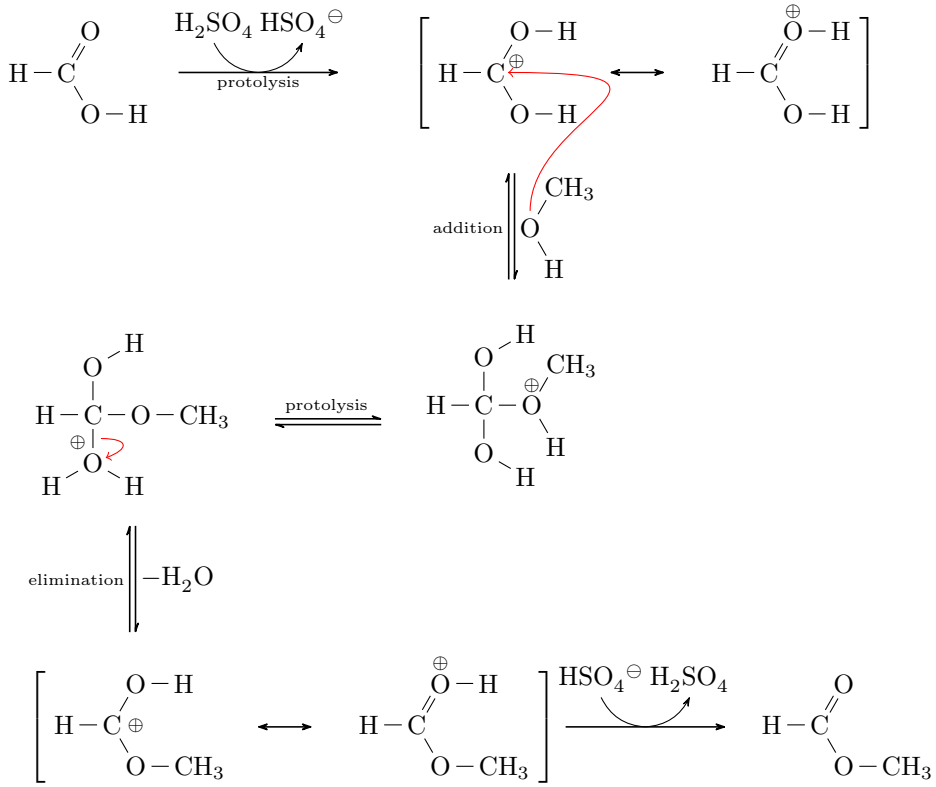
```
\begin{rxnscheme}{Hydratisation}
 \reactant[,carbonyl_A]{\chemfig{R_2C=O}}
 \anywhere{above=of carbonyl_A}{\chemfig{H-[:-30]O-[:30]H}}
 \arrow[,<=>]{\tiny slow}{}
 \transition[,transition_A]{\chemfig{R_2C(-[2,,2,,densely dotted]\chemabove{O}{\delp}(-[:150]H)-[:30]H)-[:-30,1.15,,,lddbond]O-[6,,,,densely 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}{\scriptstyle
      \oplus}H_2)-[:-60]OH}}
    \arrow[below right,<=>,.7]{$-\Hpl$}{}
    \reactant[below right]{\chemfig{R_2C(-[:60]OH)-[:-60]OH
      }}
    \arrow[below left,<=>,.7]{}{\ce{H2O}}
    \reactant[below left,zw]{\chemfig{R_2C(-[:60]OH)-[:-60]O
      |\om}}
    \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

Reaction scheme 8 Esterification



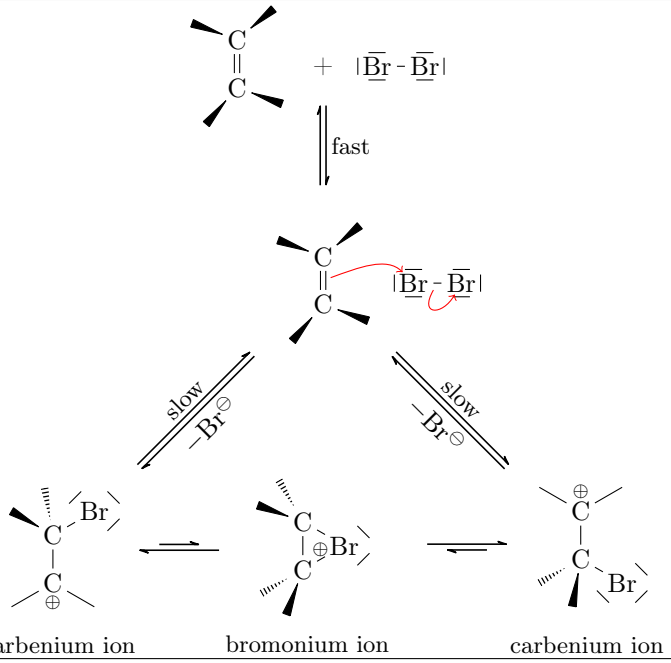

```
1  \begin{rxn}{Esterification}
2   \reactant{\chemfig{H-C(=[:60]O)-[:-60]O-H}}
3   \arrow[,-+>,1.2,protolysis]{\ce{H2SO4}}{\ce{HSO4\om}}
4   \anywhere{below=of protolysis,,yshift=1em}{\tiny
       protolysis}
5   \mesomeric{
6     \reactant{\chemfig{H-@{a2}C(-[:60]O-H)(-[:30,.5,,,draw
         =none]{\scriptstyle\oplus})-[:-60]O-H}}
7     \marrow
8     \reactant{\chemfig{H-C(=[:60]\chemabove{O}{\
         scriptstyle\oplus}-H)-[:-60]O-H}}
9   }
10  \branch[below,,xshift=-5em]{
11    \arrow[below,<=>]{\tiny addition}{\chemfig{H-[:120]@{a
         1}O-[:60]CH_3}}
12    \reactant[below]{
13      \chemfig{H-C(-[2]O-[:30]H)(-\chemabove{O}{\
```

```
            scriptstyle\oplus}(-[: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}\scriptstyle\oplus
        }(-[:-150]H)-[:-30]H}
      \elmove{b1}{0:5mm}{a3}{20:5mm}
    }
    \arrow[below,<=>]{\ce{- H2O}}{\tiny elimination}
    \mesomeric[below,,xshift=6em]{
      \reactant{\chemfig{H-C(-[:60]O-H)(-[,.5,,,draw=none]{\
        scriptstyle\oplus})-[:-60]O-CH_3}}
      \marrow
      \reactant{\chemfig{H-C(=[:60]\chemabove{O}{\
        scriptstyle\oplus}-H)-[:-60]O-CH_3}}
    }
    \arrow[,-+>,1.2]{\ce{HSO4\om}}{\ce{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

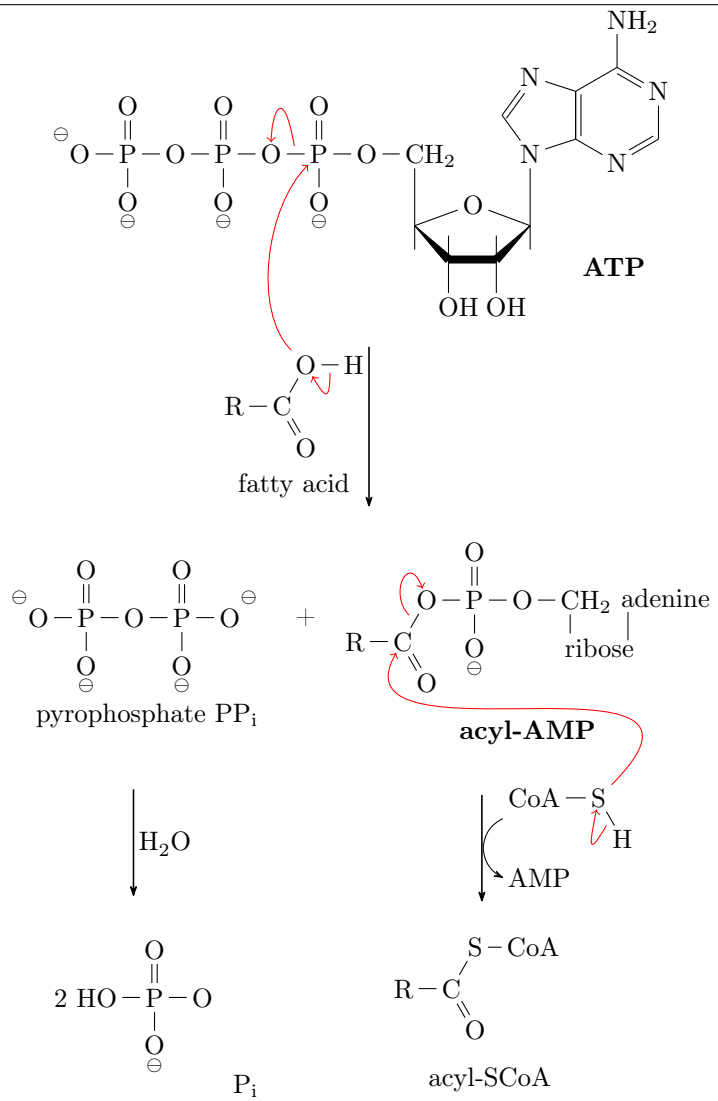



```
\begin{rxnscheme}[,H]{Electrophilic Addition}
 \setarrowlength{3em}
 \reactant{\chemfig{>[:-20]C(<[:40])=[6]C(<[:-130])<[:-20]}}
 \chemand[,plus]
 \reactant{\chemfig{\lewis{246,Br}-\lewis{026,Br}}}
 \arrow[plus.-90,<=>]{\footnotesize fast}{}
 \reactant[-90,attack]{\chemfig{>[:-20]C(<[:40])=[@{db}6]C(<[:-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]{\ce{- Br\om}}{\footnotesize slow}
 \reactant[-135,carbenium_a]{\vflipnext\chemfig{-[:-30]\chembelow{C}{\scriptstyle\oplus}(-[:30])-[6]C
```

```
      (<[:-150])(<:[:-100])-[:-30]\lewis{137,Br}}}
16  \anywhere{below=of carbenium_a}{\footnotesize carbenium
      ion}
17  \arrow[,<<=>]{}{}
18  \reactant[,bromonium]{\chemfig{>:[:-60]C?(<[:160])-[6]C
      (<[:-110])(<:[:-150])-[:30]\lewis{17,Br}?-[4,.5,,,
      draw=none]{\scriptstyle\oplus}}}
19  \anywhere{below=of bromonium,,yshift=.35em}{\
      footnotesize bromonium ion}
20  % to the right:
21  \arrow[attack.-45,<=>,2]{\footnotesize slow}{\ce{- Br\om
      }}
22  \reactant[-45,carbenium_b]{\chemfig{-[:-30]\chemabove{C
      }{\scriptstyle\oplus}(-[:30])-[6]C(<:[:-150])
      (<[:-100])-[:-30]\lewis{157,Br}}}
23  \anywhere{below=of carbenium_b}{\footnotesize carbenium
      ion}
24  \arrow[left,<<=>]{}{}
25  \mCsetup{reset}
26 \end{rxnscheme}
```

10 Activation of Fatty Acids

Reaction scheme 10 Activation of Fatty Acids

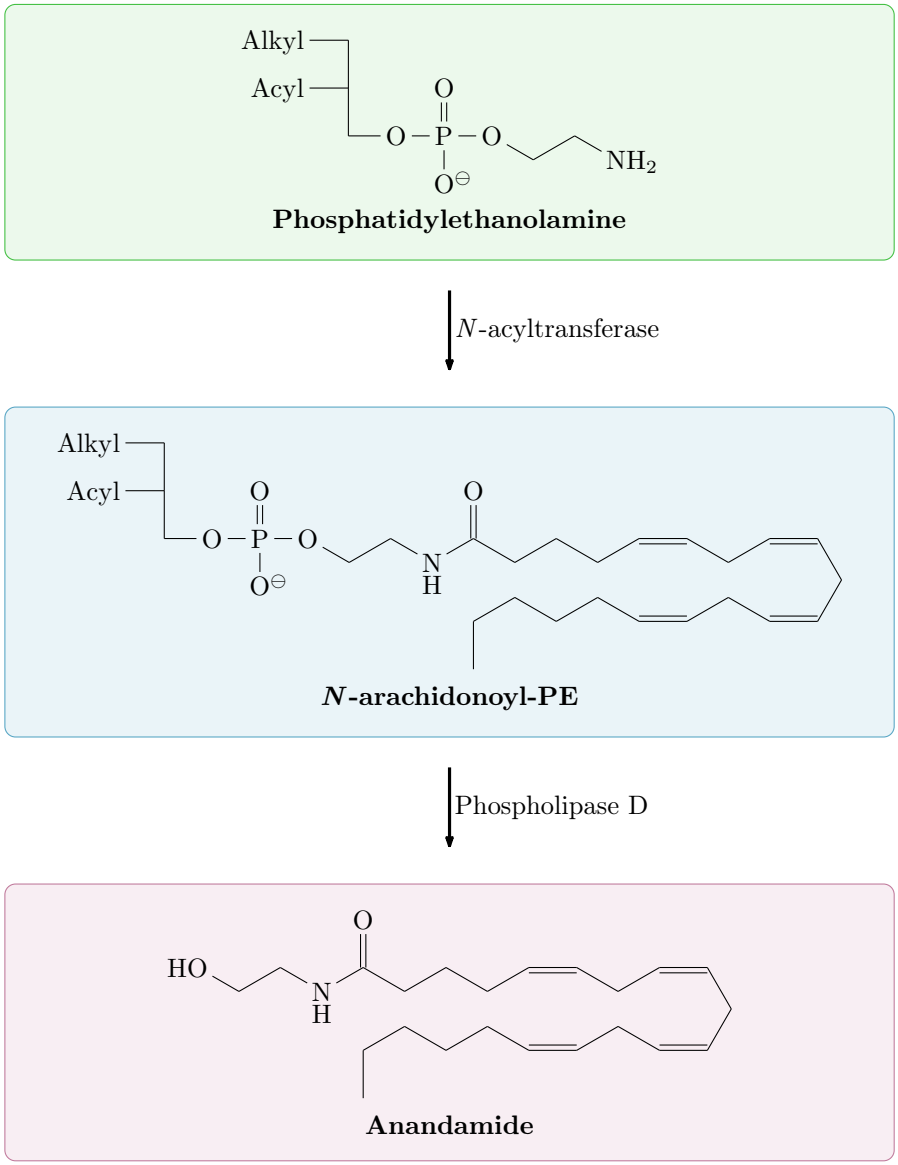



```
\def\scrom{\scriptstyle\ominus}
\begin{rxnscheme}[,H]{Activation of Fatty Acids}
 \reactant[,ATP]{\chemfig{\chemabove{O}{\hspace*{-5mm}\
    scrom}-P(=[2]O)(-[6]\chembelow{O}{\scrom})-O-P(=[2]O)
    (-[6]\chembelow{O}{\scrom})-@{O1}O-[@{b1}]@{P}P(=[2]O
    )(-[6]\chembelow{O}{\scrom})-O-CH
    _2-[6,1.5,1](-[6,.5])(-[:20,1.3]O?[a])<[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}\scrom}-P(=[2]O
        )(-[6]\chembelow{O}{\scrom})-O-P(=[2]O)(-[6]\
        chembelow{O}{\scrom})-\chemabove{O}{\hspace*{5mm
        }\scrom}}
      \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}{\scrom})(=[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]{\ce{H2O}}{}
    \reactant[below,Pi]{2~\chemfig{HO-P(=[2]O)(-[6]\
      chembelow{O}{\scrom})-O}}
    \anywhere{below right=of Pi}{P$_\text{i}$}
  }
  \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*k*Z

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



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

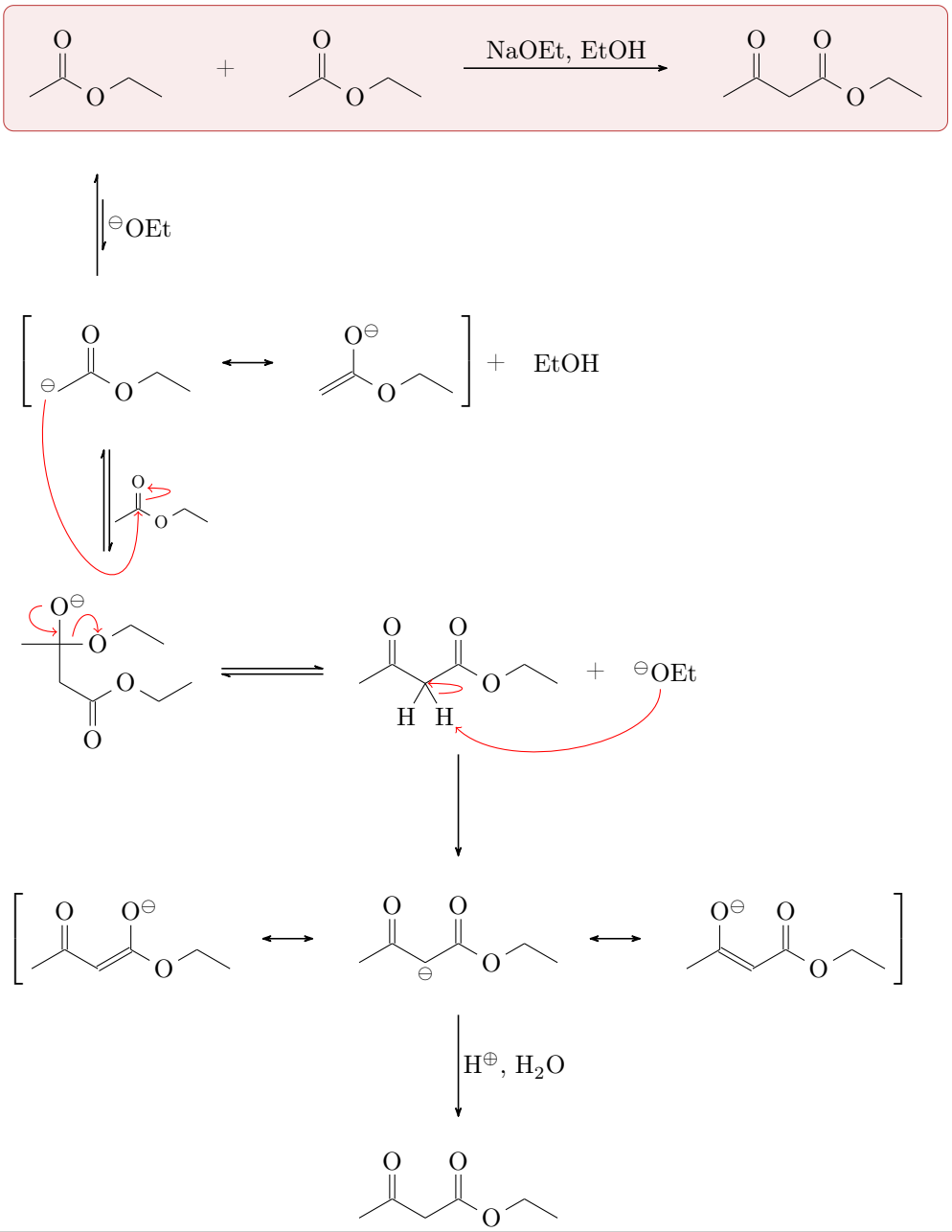
```
1  \begin{rxnscheme}{Change the layout with \TikZ}
2   \colorlet{mCgreen}{green!50!gray}
3   \colorlet{mCblue}{cyan!50!gray}
4   \colorlet{mCred}{magenta!50!gray}
```

```
  \tikzset{reactant/.style={draw=#1,fill=#1!10,minimum
     width=.8\textwidth,inner sep=1em,rounded corners}}
  \mCsetup{arrowlength=3em,arrowline=very thick}
  \reactant[,,reactant=mCgreen]{
    \chemname{\chemfig{Alky|l--[6](-[4,,,2]Acy|l)-[6]-O-P
       (=[2]O)(-[6]O|\om)-O-[:-30]-[:30]-[:-30]NH_2}}{\
       bfseries Phosphatidylethanolamine}
  }
  \arrow[below]{}{\textit{N}-acyltransferase}
  \reactant[below,,reactant=mCblue]{
    \chemname{\chemfig{Alky|l--[6](-[4,,,2]Acy|l)-[6]-O-P
       (=[2]O)(-[6]O|\om)-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\textit{N}-
       arachidonoyl-PE}
  }
  \arrow[below]{}{Phospholipase D}
  \reactant[below,,reactant=mCred]{
    \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}
  }
  \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]{\ce{NaOEt}, \ce{EtOH}}{}
   \reactant{\chemfig{[:30]-(=[2]O)-[:-30]-(=[2]O)-[:-30]
      O--[:-30]}}
```

Reaction scheme 12 Claisen-Kondensation



```
  }
  % Mechanismus:
  \branch[-90,,xshift=-13.5em]{
    \arrow[-90,<=>]{\ce{{}\om OEt}}{}
  }
  \mesomeric[-90,two,xshift=4.5em]{
    \reactant{\chemfig{[:30](-[:150,.3,,,draw=none]@{C1}\
      scriptstyle\ominus)-(=[2]O)-[:-30]O--[:-30]}}
    \marrow
    \reactant{\chemfig{[:30]=(-[2]O|\om)-[:-30]O--[:-30]}}
  }
  \chemand
  \reactant{\ce{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|\om)
    (-[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{\om @{O4}OEt}}
  \arrow[four.-90]{}{}
  \mesomeric[-90]{
    \reactant{\chemfig{[:30]-(=[2]O)-[:-30]=(-[2]O|\om)
      -[:-30]O--[:-30]}}
    \marrow
    \reactant{\chemfig{[:30]-(=[2]O)-[:-30](-[6,.3,,,draw=
      none]\scriptstyle\ominus)-(=[2]O)-[:-30]O--[:-30]}}
    \marrow
    \reactant{\chemfig{[:30]-(-[2]O|\om)=[:-30]-(=[2]O)
      -[:-30]O--[:-30]}}
  }
  \arrow[-90]{\Hpl, \ce{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}
```

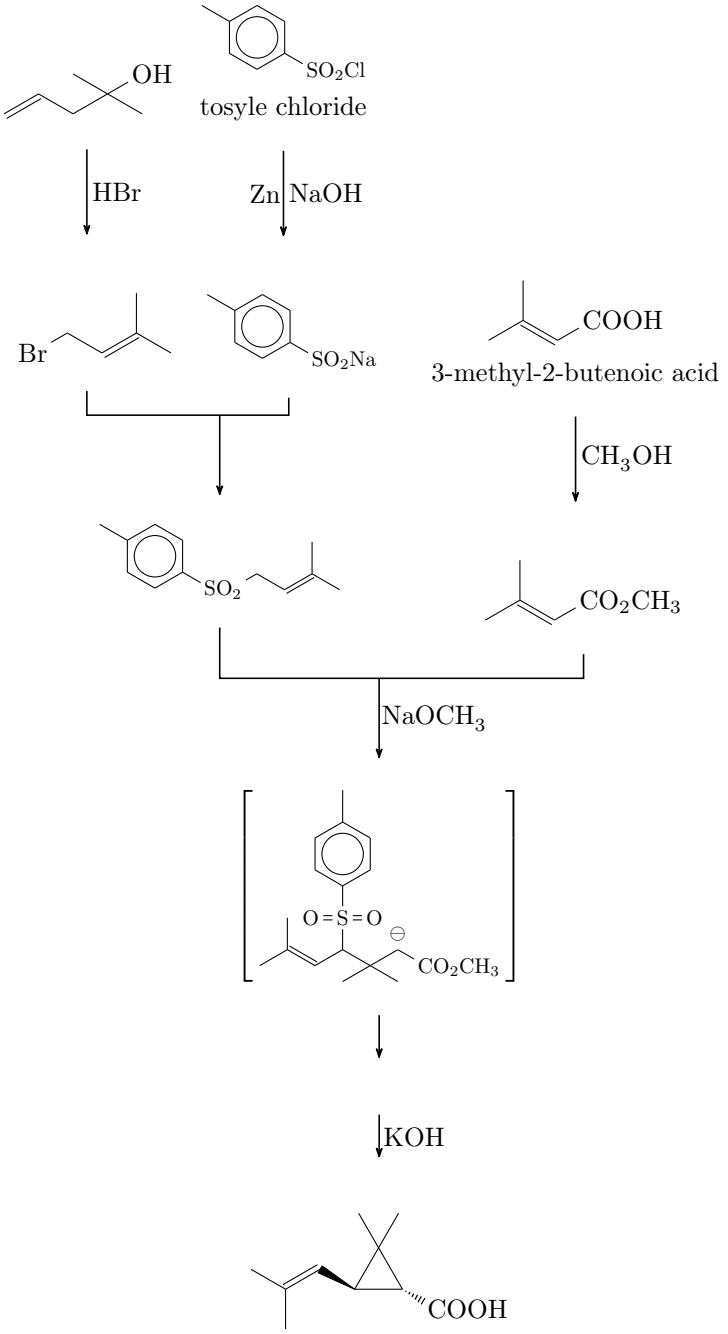
```
    \elmove{b3}{80:5mm}{O3}{90:5mm}
    \elmove{b4}{0:5mm}{C3}{0:7mm}
    \elmove{O4}{-90:1cm}{H}{-45:1cm}
  }
\end{rxnscheme}
```

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]{\ce{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_2
      Cl)---(-)-)}}{tosyle chloride}}
   \arrow[below]{\ce{NaOH}}{\ce{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}}{3-methyl-2-butenoic acid}}
   \arrow[below]{\ce{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])---(-)-)
      }}
 }
 \branch[below=of target_one,target_two,xshift=6em,yshift
    =-6em]{
   \mesomeric{\chemfig[][scale=.8]{-[::30](-[::60])
      =^[::-60]-[::60](-[::60]S(=[::90]O)(=[::-90]O)
      -[::0]**6(---(-)---))-[::-60](-[::0])(-[::-120])
```

Reaction scheme 13 Extensive Synthesis



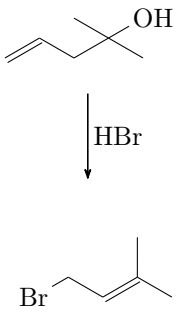
trans-chrysanthemum acid

```
        -[::60](-[::60,.5,,,white]\ominus)-[::-60]CO_2CH
        _3}}
23    \arrow[below,,.5]{}{}
24    \arrow[below,,.5]{\ce{KOH}}{}
25    \reactant[below]{\chemname{\chemfig{-[::-30](-[::-60])
        =^[::60]>[::-60](-[::90,1.2])
        -[::30,1.2](-[::120,1.2](-[::-60])-[::0])<:[::-30]
        COOH}}{\emph{trans}-chrysanthemum acid}}
26  }
27  \merge{target_one}{start_left}{start_center}
28  \merge[\ce{NaOCH3}]{target_two}{target_one}{start_right}
29 \end{rxnscheme}
```

Let's go through the code, piece by piece.

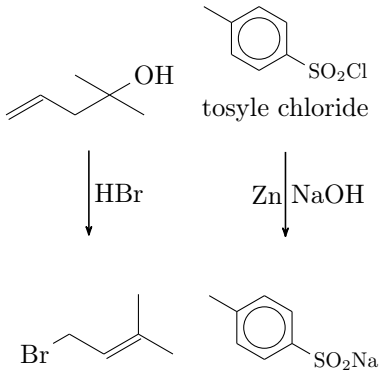
```
1  \begin{rxnscheme}[,,,.8]{Extensive Synthesis}
2   \setatomsep{1.5em}
3   \branch[,start_left]{
4     \reactant{\chemfig{=_[::30]-[::-60]-[::60](-[::-60])
        (-[::120])-[::0]OH}}
5     \arrow[below]{\ce{HBr}}{}
6     \reactant[below]{\chemfig{Br
        -[::30]-[::-60]=_[::60](-[::-60])-[::60]}}
7   }
```

In lines 1 and 2 we begin the environment and make sure, that the formulæ don't become to big. In lines 3 to 7 the first two reactants are written (lines 4 and 6) and connected with an arrow (line 5).



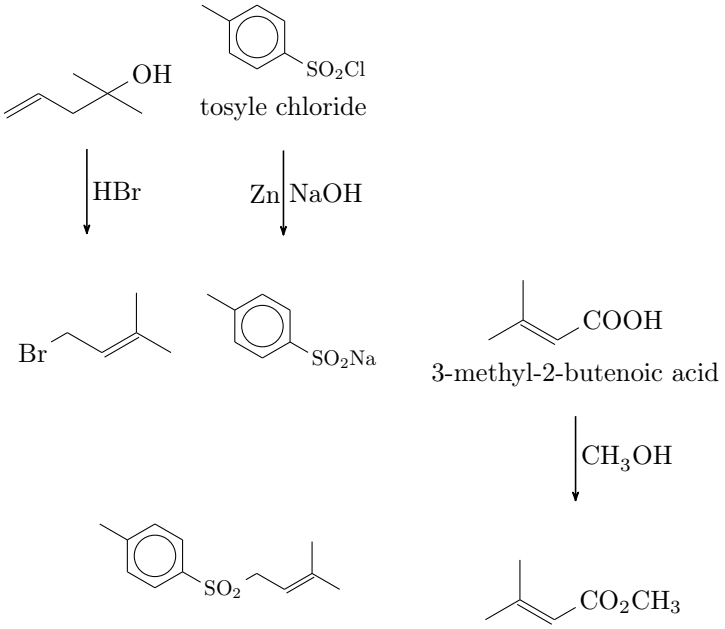

```
8   \branch[right=of start_left,start_center,yshift=1em]{
9     \reactant{\chemname{\chemfig[][scale=.8]{**6(--(-SO_2
        Cl)---(-)-)}}{tosyle chloride}}
10    \arrow[below]{\ce{NaOH}}{\ce{Zn}}
11    \reactant[below]{\chemfig[][scale=.8]{**6(--(-SO_2Na)
        ---(-)-)}}
12  }
```

In the following lines 8 to 12, we create the second branch of the synthesis.



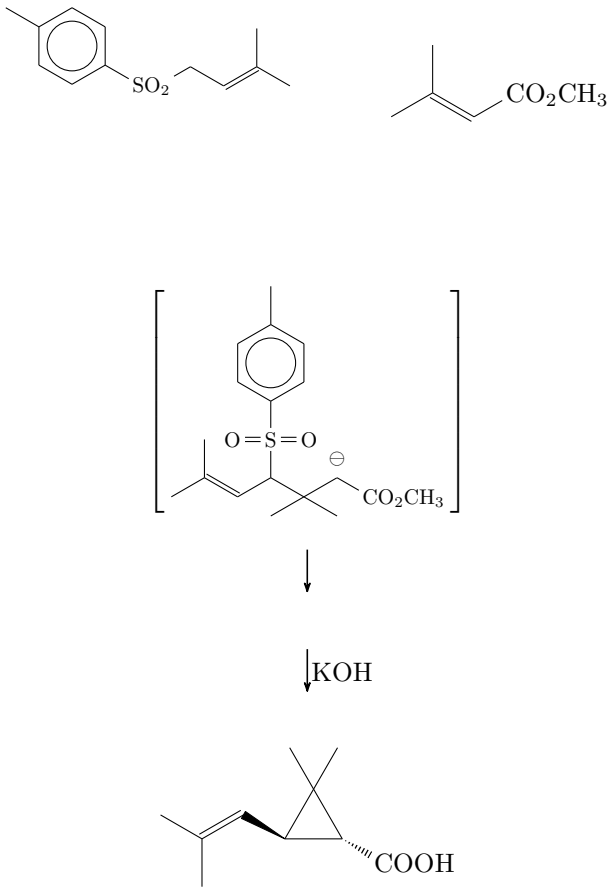

```
13    \branch[right=of start_center,start_right,xshift=3em,
        yshift=-10em]{
14      \reactant{\chemname{\chemfig{-[::30](-[::60])
          =_[::-60]-[::60]COOH}}{3-methyl-2-butenoic acid}}
15      \arrow[below]{\ce{CH3OH}}{}
16      \reactant[below]{\chemfig{-[::30](-[::60])
          =_[::-60]-[::60]CO_2CH_3}}
17    }
18    \branch[below=of start_left,target_one,xshift=5em,yshift
        =-5em]{
19      \reactant{\chemfig[][scale=.8]{**6(--(-SO
          _2-[:30]-[::-60]=_[::60](-[::60])-[::-60])---(-)-)
          }}
20    }
```

In lines 13 to 20 we create the third branch and the product of the first two branches.




```
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]\ominus)-[::-60]CO_2CH_3}}
23    \arrow[below,,.5]{}{}
24    \arrow[below,,.5]{\ce{KOH}}{}
25    \reactant[below]{\chemname{\chemfig{-[::-30](-[::-60])
         =^[::60]>[::-60](-[::90,1.2])
         -[::30,1.2](-[::120,1.2](-[::-60])-[::0])<:[::-30]
         COOH}}{\emph{trans}-chrysanthemum acid}}
26  }
```

In lines 21 to 26 we create the last branch.



trans-chrysanthemum acid

Finally, the different branches are merged, the second merging arrow gets a label and the environment is ended.

```
27    \merge{target_one}{start_left}{start_center}
28    \merge[\ce{NaOCH3}]{target_two}{target_one}{start_right}
29  \end{rxnscheme}
```