

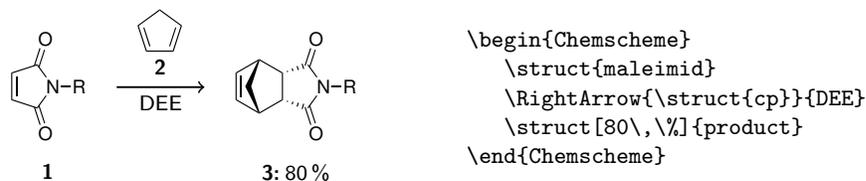
The chemschemex package*

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Abstract

The `chemschemex` package provides a comfortable method for the typesetting of (chemical) schemes based on `TikZ` code, including an automatical structure referencing.



Example 1: Chemical scheme (left) produced by a simple code (right).

Contents

1	Introduction and motivation	2
2	Usage	2
3	User commands	3
3.1	Basic commands	3
3.2	Structure commands	3
3.3	The Chemscheme environment	6
3.4	Ref commands	8
3.5	Arrows and simples	8
4	Options	10
4.1	The image option	10
4.2	The labelseparator option	10
4.3	The arrowadvance option	10

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5	Customization and advanced examples	10
5.1	Predefined TikZ styles	10
5.2	Style adjustment – some examples	13
5.3	Chemical mechanisms	14
6	Change history	15

1 Introduction and motivation

While L^AT_EX is a powerful tool for mathematical or physical issues the typesetting of chemistry derived problems is still a little bit annoying. When I wrote my thesis in organic chemistry I missed a package which produces chemical schemes as easy as you include a graphic into your document. I simply wanted to draw my structures in CHEMDRAW, include them into my document and label them.

The packages `chemscheme` and `chemnum` offer a possibility to rerender image files for this purpose. Nevertheless, they only modify a scheme that already exists. This means, that arrows, margins, alignments and other parameters cannot be defined or changed globally in your document.

By using the `TikZ` and the `fancylabel` package (which has actually been written as slave of this package) the `chemschemex` package meets all these requirements (see example 1).

2 Usage

```
\usepackage \usepackage[<options>]{chemschemex}
```

The command above will load the `chemschemex` package. It requires the packages `xkeyval`, `etextools`, `xargs`, `ifthen`, `suffix`, `TikZ`, `graphicx`, and `fancylabel`. I strongly recommend to read the documentation of the `fancylabel` package because all referencing functions are provided by this package. It contains a lot of useful options that are not described in this documentation.

3 User commands

3.1 Basic commands

`\customstruct` `\customstruct[<TikZ-capt>][<TikZ-obj>]{<capt>}{<obj>}`

The `\customstruct` command typesets the object `<obj>` in the first row of a `TikZ` matrix and the caption `<capt>` in the second row. The caption is supposed to be given as comma-separated list of label(s) and text. The two optional arguments `<TikZ-capt>` and `<TikZ-obj>` can be used to pass options to `TikZ` elements (for further information see section 5.1). All the following structure commands are based on `\customstruct`.

<code>object e.g. image</code>	<code>\customstruct[nodes={draw=blue}][draw=red]</code>
<code>label1:text</code>	<code>{{{label1:},{text}},</code>
<code>ll2:a longer text</code>	<code>{{ll2:},{a longer text}}}</code>
	<code>{object e.g. image}</code>

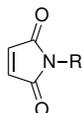
`\CSXimage` `\CSXimage[<img-opt>]{}`

The `\CSXimage` command includes the image `` using the global options `<global-img-opt>` defined by the `image` option (see section 4.1) and the options given by `<img-opt>`. This command is used in all the following structure commands and expands to `\includegraphics[<global-img-opt>,<img-opt>]{}`.

3.2 Structure commands

`\struct` `\struct[<capt>][<fam>][<img-opt>][<TikZ-capt>][<TikZ-obj>]{}`

The `\struct` command includes the image ``, sets a fancylabel (therefore it uses `` as marker and `<fam>` as family, default: `<fam>=CSX`; the use of families is described in the `fancylabel` package) and prints it. If a `<caption>` is given, it will also print the caption behind the label. The macro `\CSXlabelsep` can be changed with the `labelseparator` option.

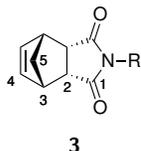


1: text

`\struct[text]{maleimid}`
expands to:
`\customstruct{{{fancylabel[CSX]{maleimid}\CSXlabelsep},{}}}`
`{\CSXimage{maleimid}}`

`\structalt` `\structalt[<capt>][<fam>][<img-opt>][<TikZ-capt>][<TikZ-obj>]{}{<alt-img>}`

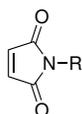
The `\structalt` command includes an image `<alt-img>` but the labeling corresponds to ``.



```
\structalt{product}{product_num}
  expands to:
\customstruct{{{fancylabel[CSX]{product}},{}}}
              {\CSXimage{product_num}}
```

`\struct*` `\struct* [<capt>] [<fam>] [<img-opt>] [<TikZ-capt>] [<TikZ-obj>] { }`
`\structalt*` `\structalt* [<capt>] [<fam>] [<img-opt>] [<TikZ-capt>] [<TikZ-obj>] { } { <alt-img> }`

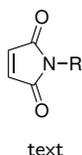
The `\struct*` and `\structalt*` commands do the same as the corresponding nonstarred versions but use `\fancylabel*` instead of `\fancylabel`. This means, that a label for this structure will be defined but not printed.



```
\struct*{maleimid}
  expands to:
\customstruct{{{fancylabel*[CSX]{maleimid}},{}}}
              {\CSXimage{maleimid}}
```

`\struct-` `\struct-[<capt>][<img-opt>][<TikZ-capt>][<TikZ-obj>]{}`

The `\struct-` command includes an image `` without any labeling.



```
\struct-[text]{maleimid}
  expands to:
\customstruct{{{},{text}}}
              {\CSXimage{maleimid}}
```

`\newstruct` `\newstruct [<sublabels>] { } { <structname> } { <Structname> } { <abbr> }`

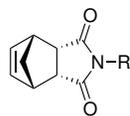
If you want to use substructures you have to define them in the preamble. The optional argument `<sublabels>` is a comma-separated list of subcaptions. Whenever you want to refer to them you just have to use their numbers. In this example the first entry ($R=H$) gets the number 1, the second entry ($R=Me$) gets the number 2 and so on. If you use a structure without substructures it is not necessary to use `\newstruct`. However, the `\newstruct` command defines the name (and Name) und abbreviation of the structure what allows you to use the commands `\structname`, `\Structname` and `\structabbr` for this structure.

```
\newstruct [ {R=H}, {R=Me}, {R=Ph} ] {product} { } { }
```

Note: All of the following structure commands assume that `\newstruct` has been used for the filename `` before.

`\Struct` `\Struct[<fam>] [<img-opt>] [<TikZ-capt>] [<TikZ-obj>]{<sublabels>}{}`

To use the `\Struct` command, the structure and its substructure have to be defined by the `\newstruct` command. It includes the image ``, sets the sublabels given in the comma-separated list of `<sublabels>` and prints each sublabel with the subcaption previously given to the `\newstruct` command (one line per sublabel).

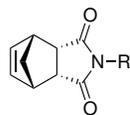


3a: R=H
3b: R=Me
3c: R=Ph

```
\Struct{1,2,3}{product}
expands to:
\customstruct{{{fancysublabel[CSX]{product}{1}\CSXlabelsep},{R=H}},
               {{fancysublabel[CSX]{product}{2}\CSXlabelsep},{R=Me}},
               {{fancysublabel[CSX]{product}{3}\CSXlabelsep},{R=Ph}}}}
{\CSXimage{product}}
```

`\Struct*` `\Struct* [<fam>] [<img-opt>] [<TikZ-capt>] [<TikZ-obj>]{<sublabels>}{}`

To use the `\Struct*` command, the structure and its substructure have to be defined by the `\newstruct` command. It includes the image `<filename>`, sets the sublabels given in the comma-separated list of `<sublabels>` and prints each sublabel without its subcaption previously given to the `\newstruct` command.



3a, c

```
\Struct*{1,3}{product}
expands to:
\customstruct{{{fancysublabel[CSX]{product}{1,3}},{}}}}
{\CSXimage{product}}
```

`\Structalt` `\Structalt [<fam>] [<img-opt>] [<TikZ-capt>] [<TikZ-obj>]{<sublabels>}{}{<alt-img>}`

Works like the `\Struct` command but includes the image `<alt-img>`. Labeling corresponds to ``.

`\Structalt*` `\Structalt* [<fam>] [<img-opt>] [<TikZ-capt>] [<TikZ-obj>]{<sublabels>}{}{<alt-img>}`

Works like the `\Struct*` command but includes the image `<alt-img>`. Labeling corresponds to ``.

`\structname` `\structname{}`

Prints the name of the structure `` that has been previously defined by the `\newstruct` command. This command is recommended for the chemical name without a leading capital letter (inside a sentence).

`\Structname` `\Structname{}`

Prints the name of the structure `` that has been previously defined by the `\newstruct` command. This command is recommended for the chemical name with a leading capital letter (at the beginning of a sentence).

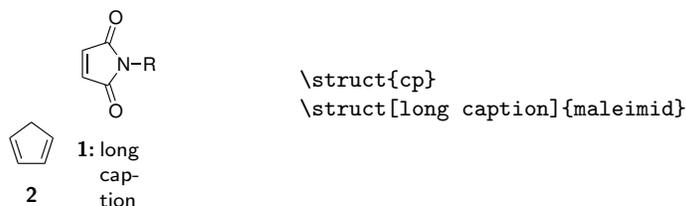
`\structabbr` `\structabbr{}`

Prints the abbreviation of the structure `` that has been previously defined by the `\newstruct` command.

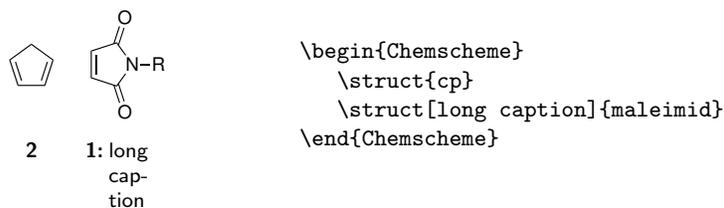
3.3 The Chemscheme environment

`Chemscheme` `\begin{Chemscheme}...structure code...\end{Chemscheme}`

If a structure command appears outside a `Chemscheme` environment each command will typeset the image and caption in its own matrix. This causes no kind of adjustment.

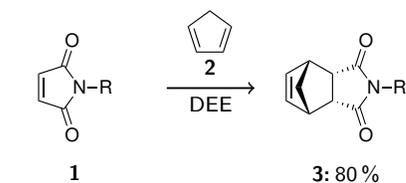


But if structure commands appear inside a `Chemscheme` environment all images and captions are printed in one matrix. This causes adjustment of the image (by default center) and the caption row (by default top) according to the `TikZ` style `CSXmatrix`.

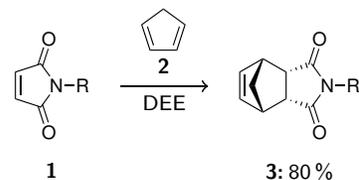
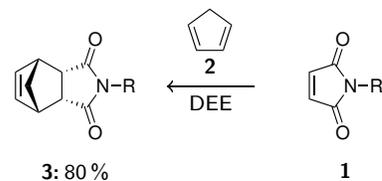


`\ChemschemeNextRow` `\ChemschemeNextRow[<row-sep>]`

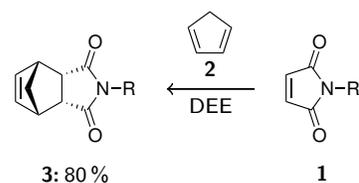
If you want to use the matrix adjustment over multiple lines you can produce a 'linebreak' using the `\ChemschemeNextRow` command. The optional argument `<row-sep>` allows you to define the space between the rows.



```
\begin{Chemscheme}
  \struct{maleimid}
  \RightArrow{\struct{cp}}{DEE}
  \struct[80\,\%]{product}
  \ChemschemeNextRow[10pt]
  \struct[80\,\%]{product}
  \LeftArrow{\struct{cp}}{DEE}
  \struct{maleimid}
\end{Chemscheme}
```

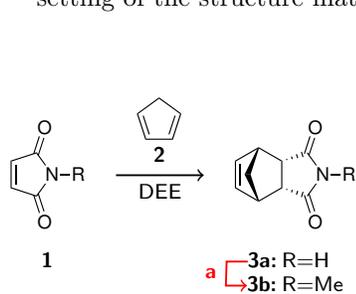


```
\begin{Chemscheme}
  \struct{maleimid}
  \RightArrow{\struct{cp}}{DEE}
  \struct[80\,\%]{product}
\end{Chemscheme}
\begin{Chemscheme}
  \struct[80\,\%]{product}
  \LeftArrow{\struct{cp}}{DEE}
  \struct{maleimid}
\end{Chemscheme}
```



`\CSXcommands` `\CSXcommands{<TikZ-code>}`

The `CSXcommands` macro allows you to draw any `TikZ` element(s) after the type-setting of the structure matrix.



```
\begin{Chemscheme}
  \struct{maleimid}
  \RightArrow{\struct{cp}}{DEE}
  \Struct{1,2}{product}
  \CSXcommands{
    \draw[->,CSXallarrows,draw=red]
      (Scheme\theCSXscheme Caption3Entry1.west) to
      ([xshift=-8pt]Scheme\theCSXscheme Caption3Entry1.west) to
      node[auto,swap,CSXlabelfont,red]{a}
      ([xshift=-8pt]Scheme\theCSXscheme Caption3Entry2.west) to
      (Scheme\theCSXscheme Caption3Entry2.west);
  }
\end{Chemscheme}
```

3.4 Ref commands

```

\structref      \structref [<fam>]{<img>}
\structref*    \structref* [<fam>]{<img>}
\structsubref  \structsubref [<fam>]{<img>}{<sublabels>}
\structsubref- \structsubref- [<fam>]{<img>}{<sublabels>}
\structsubref* \structsubref* [<fam>]{<img>}{<sublabels>}

```

The chemscemex package defines ref commands that actually do exactly what their analogs from the fancylabel package do, but with CSX as default family.¹

`\CSXstructref` The `\CSXstructref` macro allows you to change the style of all referencing commands that are shown above. The definition is shown below and may be changed as required.

```

\newcommand{\CSXstructref}[1]{%
  % #1=fancyref command
  \textbf{#1}%
}

```

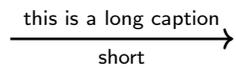
3.5 Arrows and simples

```

\customarrow \customarrow [<length>]{<style>}{<upper-capt>}{<lower-capt>}

```

The basic command for arrows is the `\customarrow` command. If the optional argument `<length>` is used, the arrow will have this length. Otherwise the arrow is stretched to the length of the widest caption advanced by the length globally defined via the `arrowadvance` option. The style argument `<style>` allows you to pass options to the TikZ `\draw` command.

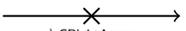
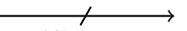
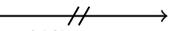
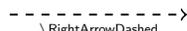
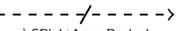
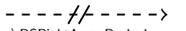
	<pre> \customarrow{->,line width=1pt} {this is a long caption} {short} </pre>
	<pre> \customarrow[60pt] {->,CSXarrowupper/.append style={red}} {this is a long caption} {short} </pre>

```

\RightArrow  \RightArrow [<length>]{<upper-capt>}{<lower-capt>}
\<arrow-cmd> \<arrow-cmd> [<length>]{<upper-capt>}{<lower-capt>}

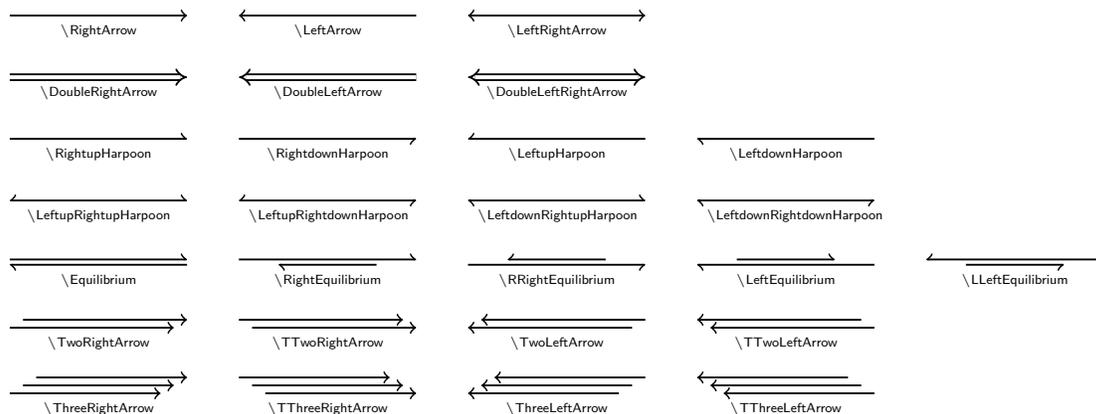
```

The table below shows a couple of arrows that are based on the `\customarrow` command. You might define some other arrows using the `\CSXdeclarearrow` command.

 <code>\RightArrow</code>	 <code>\CRightArrow</code>	 <code>\SRightArrow</code>	 <code>\DSRightArrow</code>
 <code>\RightArrowDashed</code>	 <code>\CRightArrowDashed</code>	 <code>\SRightArrowDashed</code>	 <code>\DSRightArrowDashed</code>

¹For further information please have a look into the fancylabel package documentation.

All shown arrows have a normal, a crossed out (leading C), a striked out (leading S) and a double striked out (leading DS) version of the solid and the dashed (appending Dashed) arrow.



`\CSXdeclarearrow` `\CSXdeclarearrow{<arrow-cmd>}{<style>}`

You can use the `\CSXdeclarearrow` command to declare arrows based on the `customstruct` command. The definition of `\RightArrow` is:

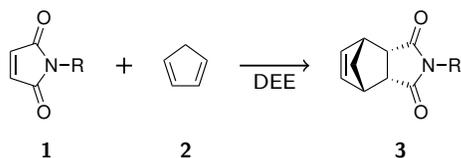
```
\CSXdeclarearrow{\RightArrow}{CSXnormalarrows,CSXRightArrow}
```

Considering the default setting of `CSXnormalarrows` and `CSXRightArrow` this means:

```
\CSXdeclarearrow{\RightArrow}{line width=0.7pt,->}
```

`\structplus` `\structplus`
`\structminus` `\structminus`

The simples (this is how I call arrow-like elements without a upper or lower caption) `\structplus` and `\structminus` can be used like any structure or arrow command:



```
\begin{Chemscheme}
  \struct{maleimid}
  \structplus
  \struct{cp}
  \RightArrow{{DEE}}
  \struct{product}
\end{Chemscheme}
```

4 Options

4.1 The image option

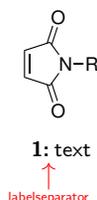
`image=` `\usepackage[image={<global-img-opt>}]{chemscheme}`

All structure commands except `\customstruct` internally use the `\CSXimage` command to include pictures with `\includegraphics`. The `image` option allows you to define options that will be passed to any image that is inserted via `\CSXimage`. The default value is `image={scale=0.7}`.

4.2 The labelseparator option

`labelseparator=` `\usepackage[labelseparator=<value>]{chemscheme}`

The `<value>` given by the `labelseparator` option is set behind every `\fancylabel` inside a structure command if some text follows. The value is saved in `\CSXlabelsep`. The default value is `labelseparator={:,}`.



4.3 The arrowadvance option

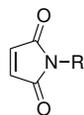
`arrowadvance=` `\usepackage[arrowadvance=<length>]{chemscheme}`

Every arrow with undefined length argument will be as long as its widest caption plus the length given by the `arrowadvance` option. This is also the minimal length of an arrow (when no captions are given). The default value is `arrowadvance=10pt`.

5 Customization and advanced examples

5.1 Predefined TikZ styles

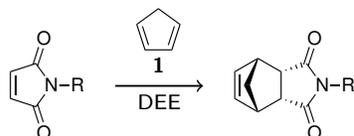
There are a lot of `TikZ` styles that are already defined by the `chemscheme` package. The following two examples show the code that is generated by `chemscheme` and hopefully help you to understand the function of each style. Some of them can be changed (**green**), some of them must not be changed (**red**) to prevent strange results or even errors. If you want to change fonts please use the **blue** coloured styles instead of appending `font=` to any style since this will cause wrong calculations. The **orange** entries are styles that are optional arguments of `\customstruct`.



```
\customstruct{{{text}}}{\CSXimage{maleimid}}
```

text

```
\begin{tikzpicture}[CSX]
  \matrix [CSXmatrix]{
    % Image row
    \node[<TikZ-obj>]
      (Scheme1Image1)
      {\CSXimage{maleimid}};\
    % Caption row
    \node(Scheme1Caption1)
      {\tikz[CSXcaption,<TikZ-capt>]
        {\node[CSXtextfont,CSXsettextwidth,CSXcaptionTextOnly]
          (Scheme1Caption1Entry1)
          {text};
        }
      };\
  };
\end{tikzpicture}
```



text

label 1text 1
label 2text 2
text 3

```
\begin{Chemscheme}
  \customstruct{{{text}}}{\CSXimage{maleimid}}
  \RightArrow{\customstruct{{{1},{}}}{\CSXimage{cp}}}{DEE}
  \customstruct{{{label 1},{text 1}},
    {{label 2},{text 2}},
    {text 3}}
    {\CSXimage{product}}
\end{Chemscheme}
```

```
\begin{tikzpicture}[CSX]
  \matrix [CSXmatrix]{
    % Image row
    \node[<TikZ-obj>]
      (Scheme1Image1)
      {\CSXimage{maleimid}};&
    \node(Scheme1Image2)
      {\hbox to <arrowlength>{}};&
    \node[<TikZ-obj>]
      (Scheme1Image3)
      {\CSXimage{product}};\
    % Caption row
    \node(Scheme1Caption1)
      {\tikz[CSXcaption,<TikZ-capt>]
        {\node[CSXtextfont,CSXsettextwidth,CSXcaptionTextOnly]
```

```

(Scheme1Caption1Entry1)
{text};
}
};&
\node(Scheme1Caption2)
{};&
\node(Scheme1Caption3)
{\tikz[CSXcaption,<TikZ-capt>]
{\node[CSXlabelfont,CSXsetlabelwidth,CSXcaptionLabelandText,
rectangle split,rectangle split horizontal,
rectangle split parts=2,rectangle split part align=base,
every two node part/.style={CSXtextfont,CSXsettextwidth}]
(Scheme1Caption3Entry1)
{label 1\nodepart{two}text 1};
\node[CSXlabelfont,CSXsetlabelwidth,CSXcaptionLabelandText,
rectangle split,rectangle split horizontal,
rectangle split parts=2,rectangle split part align=base,
every two node part/.style={CSXtextfont,CSXsettextwidth}
below left=of Scheme1Caption3Entry1.one split south,
anchor=one split north]
(Scheme1Caption3Entry2)
{label 2\nodepart{two}text 2};
\node[CSXtextfont,CSXsettextwidth,CSXcaptionTextOnly%
below=of Scheme1Caption3Entry2.south]
(Scheme1Caption3Entry3)
{text 3};
}
};\
};
\draw[CSXallarrows,CSXRightArrow,text width=(<arrowlength>-\CSXarrowadvance)]
([CSXshiftA]Scheme1Image2.west) to
node(Scheme1Image2Upper)
[CSXarrowfont,CSXarrowupper,auto]
{\tikz[remember picture,CSXStructInArrow]
{\node[<TikZ-obj>]
(Scheme1Image2UpperImage1)
{\CSXimage{cp}};
\node[below=of Scheme1Image2UpperImage1]
(Scheme1Image2UpperCaption1)
{\tikz[CSXcaption,<TikZ-capt>]
{\node[CSXlabelfont,CSXsetlabelwidth,
CSXcaptionLabelandText,rectangle split,
rectangle split horizontal,
rectangle split parts=2,
rectangle split part align=base,
every two node part/.style={
CSXtextfont,
CSXsettextwidth
}]}
(Scheme1Image2UpperCaption1Entry1)

```

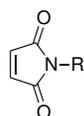
```

    {1\nodepart{two}};
    }
  };
}
}
node(Scheme1Image2Lower)
  [CSXarrowfont,CSXarrowlower,auto,swap]
  {DEE}
  (([CSXshiftB]Scheme1Image2.east);
\end{tikzpicture}

```

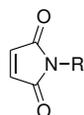
5.2 Style adjustment – some examples

As already mentioned above, please use the styles `CSXlabelfont` and `CSXtextfont` for any changes of the node font. This is necessary to ensure correct measurements. For local font adjustment of captions in structure commands use the optional argument `<TikZ-capt>`.



```
\struct[text]{maleimid}
```

1: text

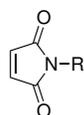


```

\struct[text]
  []
  []
  [CSXlabelfont/.style={red,font={\large}}]
  {maleimid}

```

1: text

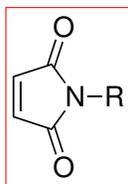


```

\struct[text]
  []
  []
  [nodes={draw=green},
  CSXtextfont/.style={blue,font={\large}}]
  {maleimid}

```

1: text

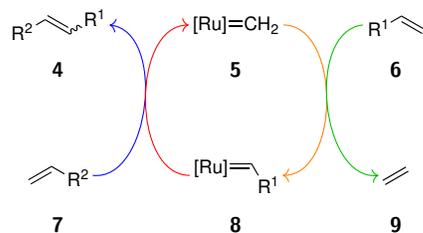


```
\struct[] [] [scale=1.5] [] [draw=red]{maleimid}
```

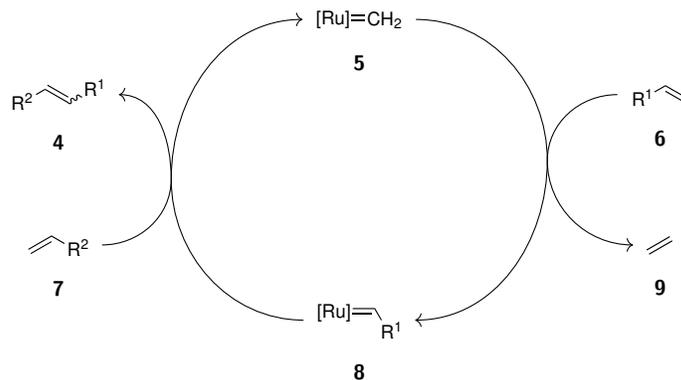
1

5.3 Chemical mechanisms

For more complex chemical mechanisms you can either use the matrix provided by the Chemscheme environment or the internal commands `\CSXimage` and `\fancylabel`:



```
\tikzset{CSXmatrix/.append style={column sep=30pt}}
\begin{Chemscheme}
  \struct{R2-CH=CH-R1}
  \struct{Ru=CH2}
  \struct{R1-CH=CH2}\ChemschemeNextRow[20pt]
  \struct{CH2=CH-R2}
  \struct{Ru=CH-R1}
  \struct{C2H4}
  \CSXcommands{
    \draw[->,draw=blue] (Scheme\theCSXscheme Image4)
      to [bend right=90,distance=22pt] (Scheme\theCSXscheme Image1);
    \draw[->,draw=red] (Scheme\theCSXscheme Image5)
      to [bend right=-90,distance=22pt] (Scheme\theCSXscheme Image2);
    \draw[->,draw=orange] (Scheme\theCSXscheme Image2)
      to [bend right=-90,distance=22pt] (Scheme\theCSXscheme Image5);
    \draw[->,draw=green!75!black] (Scheme\theCSXscheme Image3)
      to [bend right=90,distance=22pt] (Scheme\theCSXscheme Image6);
  }
\end{Chemscheme}
```



```
\tikz[node distance=1pt,mycaption/.style={CSXlabelfont}]{
  \node (n) at (0,2){\CSXimage{Ru=CH2}};
```

```

\node (ncapt) [mycaption,below=of n] {\fancylabel[CSX]{Ru=CH2}};
\node (s) at (0,-2){\CSXimage{Ru=CH-R1}};
\node (scapt) [mycaption,below=of s] {\fancylabel[CSX]{Ru=CH-R1}};
\node (nw) at (-4,1){\CSXimage{R2-CH=CH-R1}};
\node (nwcapt) [mycaption,below=of nw] {\fancylabel[CSX]{R2-CH=CH-R1}};
\node (sw) at (-4,-1){\CSXimage{CH2=CH-R2}};
\node (swcapt) [mycaption,below=of sw] {\fancylabel[CSX]{CH2=CH-R2}};
\node (ne) at (4,1){\CSXimage{R1-CH=CH2}};
\node (necapt) [mycaption,below=of ne] {\fancylabel[CSX]{R1-CH=CH2}};
\node (se) at (4,-1){\CSXimage{C2H4}};
\node (ecapt) [mycaption,below=of se] {\fancylabel[CSX]{C2H4}};
\node (w) at (-2.5,0) {};
\node (e) at (2.5,0) {};
\draw [->] (s) to [out=180,in=270] (w) to [out=90,in=180] (n);
\draw [->] (n) to [out=0,in=90] (e) to [out=270,in=0] (s);
\draw [->] (sw) to [out=0,in=270] (w) to [out=90,in=0] (nw);
\draw [->] (ne) to [out=180,in=90] (e) to [out=270,in=180] (se);
}

```

6 Change history

2014/07/15 Initial version

2017/04/03 Bug within the `\Struct` command fixed