

# quickreaction

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Simple and fast way to typeset chemical reactions

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## 1 Licence

This work may be distributed and/or modified under the conditions of the L<sup>A</sup>T<sub>E</sub>X Project Public License, version 1.3c or later. The latest version of this license is at <https://www.latex-project.org/lppl.txt>.

## 2 Requirements

quickreaction needs the packages `xparse` and `tikz`. It loads tiks libraries `matrix` and `positioning`.

### 3 Motivations

The aim of this package is to provide a simple and fast way to typeset elementary chemical reactions. There are already some packages that provide many and more sophisticated ways to draw all kinds of schemes, but all of them require a lot of effort. When you try to typeset a reaction, problems arise when it is time to align all reactants and, most of all, to align their names. For simple compounds, it is not so difficult to get good results, but for larger molecules, you have to spend a lot of time in order to do it. In addition, there are many commands and environments that provide various types of arrows to use in reaction schemes, but none of them have all the necessary functions: an arrow must extend with the text, support arguments of any type, and have the ability to use parboxes for any numbered indications, which are common in chemistry.

This package is nothing else than a bunch of macros I used to create reactions in the fastest way when an incoming project is imminent, but I decided to publish it in order to help everyone who gets stuck at first and decides to switch to other programs which, even if they can be powerful reaction setters, often do not match the style of the document with different fonts, graphical styles and blurred images that, when inserted, irremediably compromise the style of the document. A chemist-proof way to create reactions may help to initiate newbies and expand the use of L<sup>A</sup>T<sub>E</sub>X in chemistry.

### 4 Options

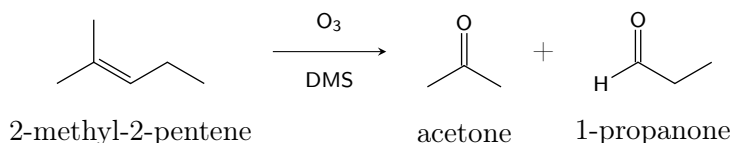
Using `chemfig` as a chemical structure drawer, the option `iupac` sets the style of bonds following what I have inferred and summarized from the [IUPAC recommendations](#). Without this option, the `chemfig` style will be the standard one. In case you want your own configuration, simply copy and paste the code below in your preamble to change it as you like. You can find the explanation of the terms and more options in the [chemfig manual](#).

```
\renewcommand{\printatom}[1]{%
\fontsize{8pt}{10pt}\selectfont{\ensuremath{\mathsf{#1}}}}
\setchemfig{
cram rectangle=false,
cram width=2.5pt,
cram dash width=0.5pt,
cram dash sep=1.5pt,
atom sep=16pt,
bond offset=1pt,
double bond sep=2pt,
bond join = true,
bond style={line width=0.5pt}
}
```

## 5 Basic Usage

This package provides the `quickreaction` environment and the command `\quickarrow`. It is based on the `TikZ matrix of nodes` and aligns all the reactants and products at the center of the TikZ box in which they are contained. For most cases, it is a sufficient setting to get good results, but to achieve perfection, one can use many other packages, for example, `chemfig` itself or `mychemistry`. An example is worth more than a thousand words:

```
%Preamble
\usepackage{xparse}
\usepackage{tikz}
\usepackage{chemfig}
\usepackage[iupac]{quickreaction}
%Document
\begin{quickreaction}
\chemfig{[:30]-(-[:90])=[:-30]--[:-30]} \& \quickarrow[\chemfig{0_3}][\%
\chemfig{DMS}] \& \chemfig{[:30]-(-[:90])=[:-30]0} \& + \& \chemfig{0%
=[:-30]-[:30]-[:-30]} \& \&
2-methyl-2-pentene \& \& acetone \& \& 1-propanone \&
\end{quickreaction}
```



The structure of the reaction simply follows the TikZ matrix syntax: the separator between cells is `\&` and for rows is `\\`. I changed the cell separator from the standard `&` to `\&` to avoid beamer issues.

The `\quickarrow` command has two optional arguments: one for the label above and one for the label below. The minimum arrow length is set at 1 cm.

`\quickarrow[label above][label below]`

## 6 Advises for Ultra-fast Reaction Typeset

As far as I know, with the introduction of this package, the combo `mol2chemfig` and `quickreaction` can lead to the fastest way to draw chemical reactions with  $\text{\LaTeX}$ . `mol2chemfig` is a Python program that generates the `chemfig` code just from the SMILES (Simplified Molecular Input Line Entry System), which can be obtained from any graphical software for drawing molecules or from any online database. The unofficial version available for Python3 is downloadable at <https://pypi.org/project/mol2chemfigPy3/>. To obtain the `chemfig` string, I usually use the command

```
mol2chemfig -zwf -i direct "SMILES"
```

Once obtained, the chemfig code can be slapped into the `quickreaction` environment without any knowledge of what you are doing, but obtaining almost instantly the desired result.

## 7 Examples

Chemfig string can be very long so in the next examples I will create a macro for every compound with a `\newcommand` in the preamble in order to keep the environment clean and to focus on the examples aspects.

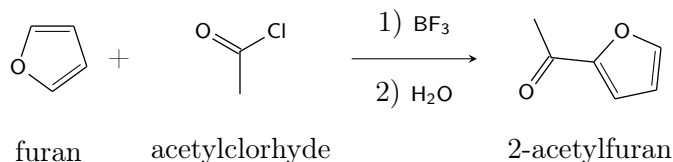
### 7.1 Labels Aligment

It is common in chemistry to specify the order of multiple separate steps in a reaction.

```
%Preamble
\usepackage{xparse}
\usepackage{tikz}
\usepackage{chemfig}
\usepackage{mol2chemfig}
\usepackage[iupac]{quickreaction}

%C1=COC=C1
\newcommand{\furan}{\chemfig{-[:180,,,dbl={73}{73}]-[:252]O-[:324]-[:36,,,%
  dbl={73}{73}]-[:108])}}
%CC(=O)C1
\newcommand{\acetylclorhyde}{\chemfig{-[:90](=[:150]O)-[:30]C1}}
%CC(=O)C1=CC=C1
\newcommand{\acetylfuran}{\chemfig{-[:294](=[:234]O)-[:354]-[:300,,,dbl%
  ={:73}{73}]-[:12]-[:84,,,dbl={73}{73}]-[:156]O(-[:228])}}

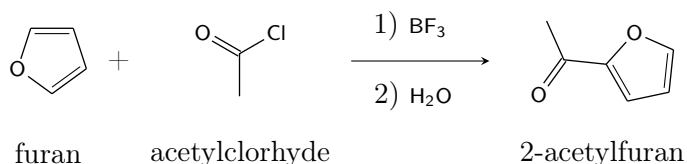
%Document
\begin{quickreaction}
\color{red}furan \& + \color{red}\acetylclorhyde \color{red}\quickarrow[1] \chemfig{BF_3}[2]\chemfig{H%
  _2O} \color{red}\acetylfuran \\
\color{red}furan \color{red}\& \color{red}acetylclorhyde \color{red}\& \color{red}2-acetylfuran \\
\end{quickreaction}
```



Usually, when there are no steps, arrow labels above and below are centered but when there are multiple steps labels are left aligned, as in a list. In the above example labels are

centered by default and the numbers result not correctly aligned. The use of a properly sized `\parbox` solves the problem:

```
\begin{quickreaction}
\furan \& + \& \acetylchlorhyde \& \quickarrow[\parbox{1.2cm}{1} \chemfig{BF%
_3}]] [\parbox{1.2cm}{2} \chemfig{H_2O}]] \& \acetylfuran \&
\end{quickreaction}
```



## 7.2 Multiple Labels

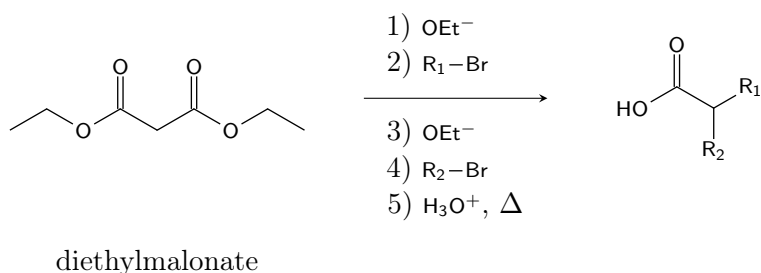
Similarly to the previous example, reactions with multiple consecutive steps can be set using `\parbox`.

```
%Preamble
\usepackage{xparse}
\usepackage{tikz}
\usepackage{chemfig}
\usepackage[iupac]{quickreaction}

%C(CC(=O)OCC)(=O)OCC
\newcommand{\diethylmalonate}{\chemfig{-[:30]-[:30]O-[:30](=[:90]O)%
-[:30]-[:30](=[:90]O)-[:30]O-[:30]-[:30]}}
\newcommand{\malonicproduct}{\chemfig{HO-[:30](=[:90]O)-[:30](-[:90]R_2)%
-[:30]R_1}}

%Document
\begin{quickreaction}
\diethylmalonate \& \quickarrow[\parbox{1.8cm}{1} \chemfig{OEt~{-}}] \& 2) \&
\chemfig{R_1-Br}} [\parbox{1.8cm}{3} \chemfig{OEt~{-}}] \& 4) \chemfig{R_2-%
Br} \& 5) \chemfig{H_3O~{+}}, $\Delta$] \& \malonicproduct \&
\end{quickreaction}
```





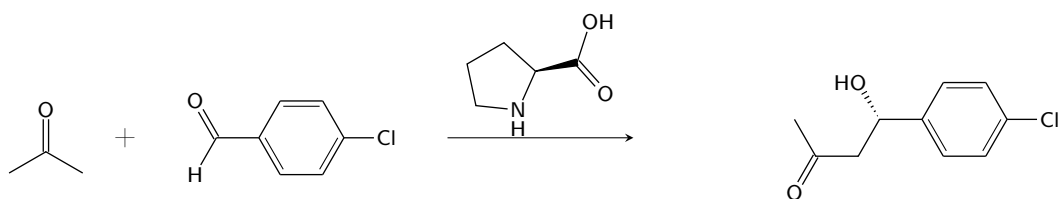
## 7.4 Auto-adjusting Column Spacing for Large Labels

When the above arrow label is higher than the depth of the deepest molecule, molecules names get shifted down to preserve the symmetry of the entire reaction box.

```
%Preamble
\usepackage{xparse}
\usepackage{tikz}
\usepackage{chemfig}
\usepackage{mol2chemfig}
\usepackage[iupac]{quickreaction}

%CC(=O)C
\newcommand{\acetone}{\chemfig{-[:90](-[:150])=[:30]O}}
%C1=CC(=CC=C1C=O)C1
\newcommand{\chlorobenzaldehyde}{\chemfig{O=[:300](-[:120]H)--[:300,,,dlh%
]--[:60,,,dlh](-C1)-[:120]-[:180,,,dlh](-[:240])}}
%C1C[C@H](NC1)C(=O)O
\newcommand{\Lproline}{\chemfig{O=[:132](-[:72,,,1]OH)%
>[:192]-[:138]-[:210]-[:282]-[:354]\mcfbelow{N}{H}(-[:66])}}
\newcommand{\clhydroxybutanone}{\chemfig{-[:300](=[:240]O)%
--[:60](<[:120,,,2]HO)--[:300,,,dlh]--[:60,,,dlh](-C1)%
-[:120]-[:180,,,dlh](-[:240])}}

%Document
\begin{quickreaction}
\acetone \& + \& \chlorobenzaldehyde \& \quickarrow[\Lproline] \& \%
clhydroxybutanone\
\acetone \& \& 4-chlorobenzaldehyde \& \& 4-(4-chlorophenyl)-4-hydroxy-2-%
butanone \
\end{quickreaction}
```

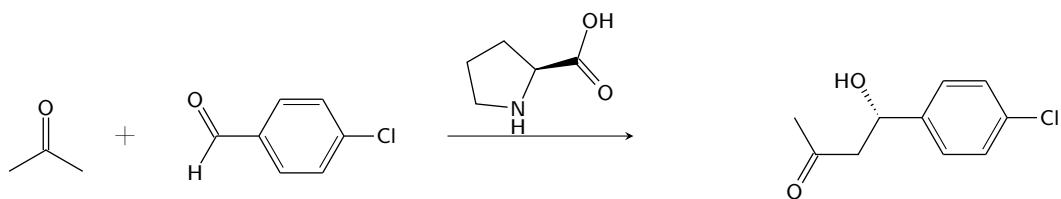


acetone      4-chlorobenzaldehyde

4-(4-chlorophenyl)-4-hydroxy-2-butanone

To replace them at their standard distance, add the deepest molecule and the entire `\quickarrow[\Lproline]` as two optional argument of the environment to compute and store the negative shift to apply and specify the stored length with `\fixrow`.

```
%Document
\begin{quickreaction}[\quickarrow[\Lproline]][\clhydroxybutanone]
\acetone \& + \& \chlorobenzaldehyde \& \quickarrow[\Lproline] \& \%
\clhydroxybutanone\\[\fixrow]
acetone \& \& 4-chlorobenzaldehyde \& \& 4-(4-chlorophenyl)-4-hydroxy-2-%
butanone \\
\end{quickreaction}
```



acetone      4-chlorobenzaldehyde

4-(4-chlorophenyl)-4-hydroxy-2-butanone