Chemical expressions

Drawing chemical equations using \chemfig package.

Bonds:

\documentclass{article}
\usepackage{chemfig}
\begin{document}
\chemfig{H-C(-[2]H)(-[6]H)-C(=[1]0)-[7]H}
\end{document}

$$H \longrightarrow C \longrightarrow C$$

Bond types

Bond type	Code	output
Single	\chemfig{O - H}	О—Н
Double	$\left(0 = H\right)$	О —— Н
Triple	\chemfig{0 ~ H}	о==н
plain right cram	\chemfig{0 > H}	О
plain left cram	\chemfig{0 < H}	ОЩН
dashed right cram	\chemfig{0 >: H}	Olim. H
dashed left cram	\chemfig{0 <: H}	О чиПН

hollow right cram	\chemfig{0 > H}	ОСН
hollow left cram	\chemfig{0 < H}	О≪Н

Arrows

\leftarrow	\leftarrow	\Leftarrow	\Leftarrow
\rightarrow	\rightarrow	\Rightarrow	\Rightarrow
\leftrightarrow	\leftrightarrow	\rightleftharpoons	\rightleftharpoons
\uparrow	\uparrow	\downarrow	\downarrow
11	\Uparrow	1	\Downarrow
\Leftrightarrow	\Leftrightarrow	1	\Updownarrow
\mapsto	\mapsto	\longmapsto	\longmapsto
7	\nearrow	A	\searrow
~	\swarrow	^	\nwarrow
	\leftharpoonup		\rightharpoonup
_	\leftharpoondown	$\overline{}$	\rightharpoondown

Latex code:

 $1 + Cl_2 \rightarrow 2HCl$

$$2H + Cl_2 \rightarrow 2HCl$$

Angles

There are several ways to define angles to draw the bonds between molecules.

To define chemical formulae you can use units that define the angles

 $\left(A-[1]B-[7]C\right)$

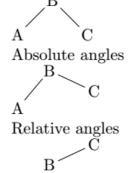
Absolute angles

\chemfig{A-[:50]B-[:-25]C}

Relative angles

\chemfig{A-[::50]B-[::-25]C}

To define chemical formulae you can use units that define the angles



Each one of the three commands in the example above uses a different method to determine the angle between bonds.

• **default units** In the command \chemfig{A-[1]B-[7]C} the parameters inside brackets set the angle in special units, each unit equals 45°. Hence in the example the angles are 45° and 315°.

- **absolute units** The angles can be set in absolute units, in the command \ chemfig{A-[:50]B-[:-25]C} the parameter inside the brackets represent the angle, in degrees, measured from the horizontal baseline. Negative angles are allowed.
- *relative angles* In the third example \chemfig{A-[::50]B-[::-25]C} the angles are measured from the previous bond, instead of the baseline.

Rings:

The example below presents the syntax to draw regular polygons

Latex code:

Regular polygons
\chemfig{A*5(-B=C-D-E=)}
Incomplete rings are also possible
\chemfig{A*5(-B=C-D)}

Regular polygons



Incomplete rings are also possible



The syntax of the command $\left(A*5(-B=C-D-E=)\right)$ is explained below:

A

This is the first atom, the rest of the atoms will be drawn from here

*5

Number of sides of the polygon

(-B=C-D-E=)

The rest of the atoms and bonds. If not enough are passed to complete the polygon, an incomplete ring will be drawn.

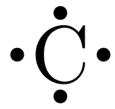
There is an additional parameter that can be passed to this command, a double asterisk. For instance, if "**5" is set instead of "*5" a circle is drawn inside the polygon.

Lewis Structures

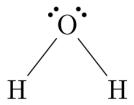
syntax \lewis{<n1><n2>...<ni>,<atom>}

Lewis structures use the syntax \lewis{<n1><n2>...<ni>,<atom>}, where <ni> is a number between 0 and 7 representing the position of the electrons. By default, the electrons are represented by a dash (-). Appending a period (.) or colon (:) after a number will displaysingle and paired electrons respectively.

\lewis{0.2.4.6.,C}



\chemfig{H-[:52.24]\lewis{1:3:,0}-[::-104.48]H}



Practice exercises for chemical equations

$$\rm M_2O_2 + 2H_2O \to 2M^+ + 2\,OH^- + H_2O_2$$

$$CO_3^{2-} + H_2O \rightarrow HCO_3^- + OH^-$$

$$\mathrm{BeO} + \mathrm{C} + \mathrm{Cl}_2 \xrightarrow{ 600-800 \mathrm{K}} \mathrm{BeCl}_2 + \mathrm{CO}$$

$$CaCO_3 \xrightarrow{heat} CaO + CO_2$$

$$\begin{array}{c} \text{CH}_3 \\ \mid \\ \text{CH}_3 - \text{C} - \text{CH} - \text{CH}_2 - \text{CH}_3 \\ \mid \quad \mid \\ \text{CH}_3 \quad \text{C}_2 \text{H}_5 \end{array}$$

$$\begin{array}{ccc} & & & & \text{CH}_3\\ \text{CH}_3 - \text{C} = \text{CH}_2 + \text{H}_2\text{O} & \xrightarrow{\text{H}^+} & \text{C} - \text{CH}_3\\ \text{CH}_3 & & & \text{CH}_3 & \text{OH} \end{array}$$

$$H_{2}C$$
 N
 $C=O$
 $H_{2}C$
 CH_{2}
 $H_{2}C$
 CH_{2}

$$\begin{array}{cccc} & & & & & & OH \\ & & & & & & & \\ & + CH_2O & & \xrightarrow{\overline{O}H} & & & & \\ \end{array}$$

$$\stackrel{\cdot \cdot \cdot}{N}=N=\stackrel{\cdot \cdot \cdot}{O} \longleftrightarrow :N\equiv N-\stackrel{\cdot \cdot \cdot}{O}:$$