

Drawing 2D chemical structures in L^AT_EX with chemfig

1. Basics – aspirin

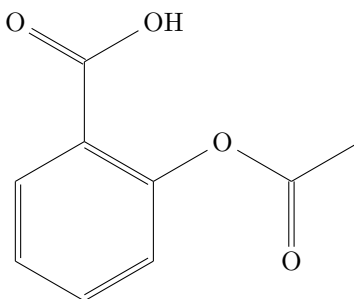
The package `chemfig` lets you draw chemical structures directly in your L^AT_EX documents without the need for creating images with other software packages and then importing them into your manuscript.

Assuming you have the `chemfig` package as part of your L^AT_EX installation (most modern installations such as T_EX Live should already include this package) simply add

```
\usepackage{chemfig}
```

to the header of your L^AT_EX document and this will also automatically load the `tikz` graphics package which does the 'background' work for `chemfig`.

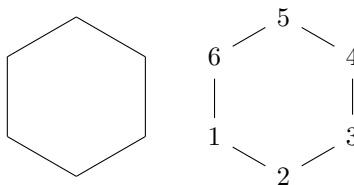
We can start with a fairly simple molecule – aspirin:



2-Acetoxybenzoic acid (aspirin)

There are several ways to begin drawing the aspirin molecule but let's start with the six-membered ring. The basic structure is drawn with the following code

```
\chemfig{*6(-----)}
```

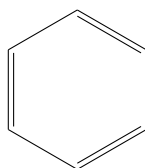


Cyclohexane

The `*` tells `chemfig` that the structure is going to be a ring and the number following it defines the number of atoms in the ring. `chemfig` numbers the atoms from the lower left position (shown in the figure on the right). This will be important when we come to add substituents later.

The hyphens (-) tell `chemfig` that all the bonds will be single. In order to add double bonds we can substitute the equal (=) sign for some of the hyphens and obtain the benzene structure

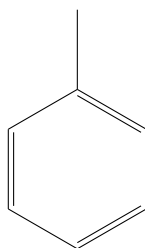
```
\chemfig{*6(==--==)}
```



Benzene

Now that we have the benzene core we can start to build up the rest of the aspirin molecule. As it is formally a benzoic acid derivative we can start with the carboxylic acid group. We begin by adding a side chain to the top position in the ring which gives us toluene. To do this we need to add a hyphen in parentheses so that `chemfig` knows that this new single bond is a side chain and not part of the ring:

```
\chemfig{*6(==--=(-)--)}
```



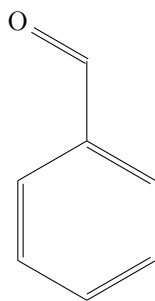
Toluene

So far we have been able to draw our structure without specifying anything about bond angles because `chemfig` knows the correct angles for rings and first substituents but now we need to tell it how we want the additional substituents to be added. To set the angle that a new bond makes at its source atom we need to add information in square brackets before the bond.

There are two possibilities for the bond angle. We can make it an *absolute* angle by placing the number of degrees in position 1 after a single colon in the brackets `[:60]` and this would fix the bond to be at 60 degrees with respect to the page. Alternatively (and generally more useful) we can place the number in position 2 after two colons `[:,60]` which defines an angle with respect to the preceding bond. Such *relative* angles are maintained even if we rotate the molecule or perform other operations. If we use an *absolute* angle and rotate the molecule that bond will remain where it is in relation to the page axis.

To make the carboxylic acid group we will need to add an OH group and an O atom with bond angles of 60° . We begin with the double-bonded O atom so as to produce benzaldehyde (although we could just have easily started with the OH).

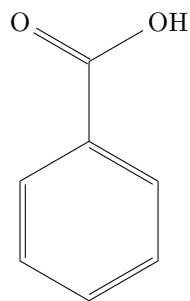
```
\chemfig{*6(---(=[:60]O)---)}
```



Benzaldehyde

Now we can add the OH group. Bear in mind that it will have to have an angle of -60° relative to the attachment atom.

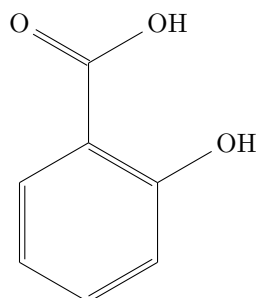
```
\chemfig{*6(---(-[: -60]-OH)=[:60]O---)}
```



Benzoic acid

Now that we have our benzoic acid we can start to build up the second side chain and we will begin by adding an OH to ring position 4 to make a precursor to aspirin, the natural product salicylic acid.

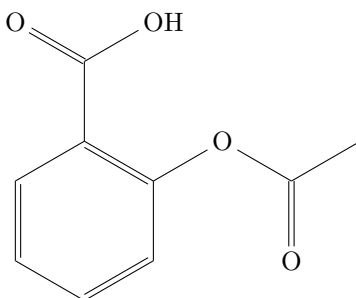
```
\chemfig{*6(---(-OH)=(-[: -60]-OH)=[:60]O---)}
```



2-Hydroxybenzoic acid (salicylic acid)

The final step we have to perform is to change this OH group to a methyl ester. Again we will use relative angles to define the orientation of the added bonds.

`\chemfig{*6(==(-0-[: -60] ([: -60]=O)-)=(-[: -60]OH)=[: 60]O)-=)}`



2-Acetoxybenzoic acid (aspirin)

We now have the completed molecular structure of aspirin encoded in a single line of text that can easily be included in any manuscript written using L^AT_EX.