

Drawing 2D chemical structures in L^AT_EX with chemfig

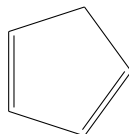
2. Custom substructures

In this tutorial we will continue to use the chemfig package to draw chemical structures in L^AT_EX. We begin by adding the following to the preamble of our L^AT_EX document

```
\usepackage{chemfig}
```

This time we will be drawing more complicated molecules. Let's start with the 1,3-cyclopentadiene molecule

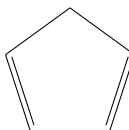
```
\chemfig{*5(-===)}
```



1,3-cyclopentadiene

To improve appearance we should rotate the molecule slightly. Note that the rotation of 18° is applied at the first atom

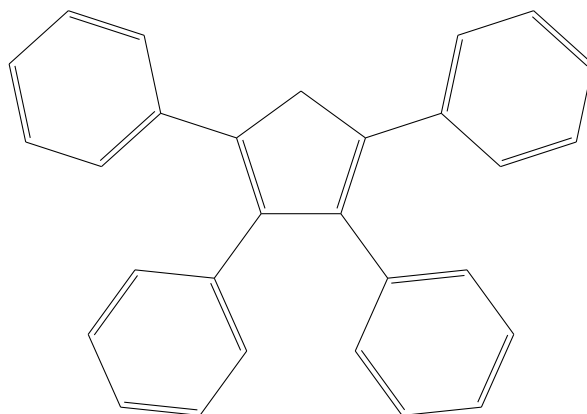
```
\chemfig{[:18]*5(-===)}
```



1,3-cyclopentadiene

To begin with, let's create a symmetrically substituted compound with four phenyl rings added to the planar carbons

```
\chemfig{[:18]*5((-*6(-====))-(*6(-====))=(*6(-====))--(*6(-====))=)}
```



1,2,3,4-tetraphenyl-1,3-cyclopentadiene

It is easy to see that using `chemfig` can rapidly become very complex and even building a symmetrical system such as 1,2,3,4-tetraphenyl-1,3-cyclopentadiene can become something of a chore. Attempting to create even more complex structures (and figure out where the inevitable errors have occurred) soon seems more trouble than it's worth.

Fortunately, `chemfig` has a neat trick to help out in situations like this. We can define re-usable subsystems and create a private shorthand to help us.

The command `\definesubmol` is used as follows to create a benzene ring which we can use on its own or as a phenyl ring substituent in larger structures

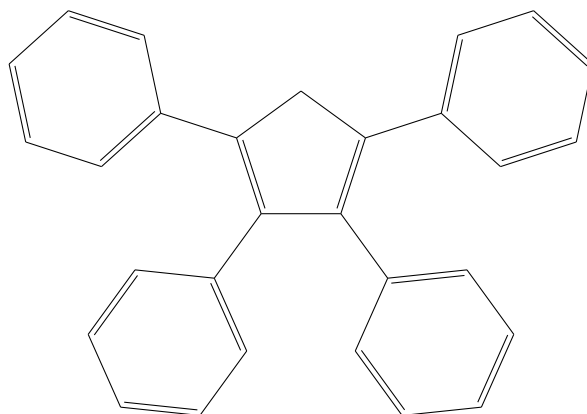
The shorthand for the fragment is given after the second backslash (`bz`) and the usual `chemfig` code for a benzene ring is given in the curly brackets

```
\definesubmol\bz{*6(====)}
```

To insert our benzene fragment into an atom position in our molecule we need to type an exclamation mark followed by the fragment name

```
\chemfig{[:18]*5((-!\bz)-(-!\bz)=(-!\bz)--(-!\bz)=)}
```

This shortened command yields the same structure as the much longer one used above but with much less typing (and possibility of errors).



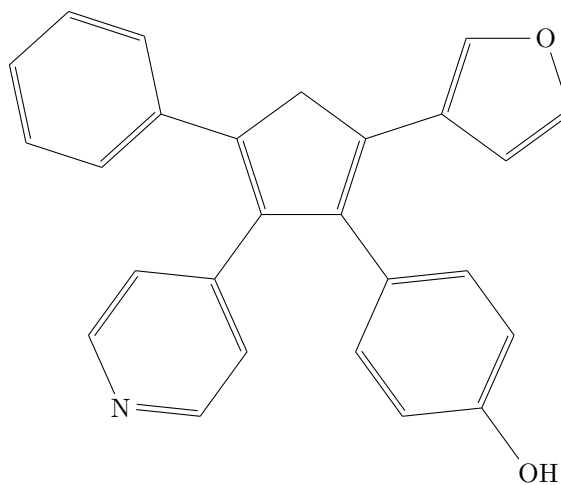
Similarly, we can define other substructures and substitute them into our structure

Pyridine: `\definesubmol\pyr{*6(==N==)}`

Phenol: `\definesubmol\bOH{*6(==(-OH)==)}`

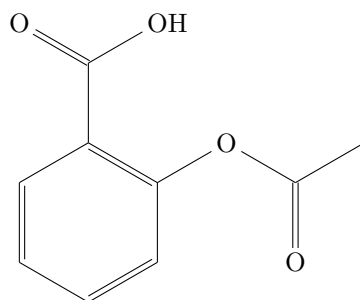
Furan: `\definesubmol\fur{*5(==O==)}`

`\chemfig{[:18]*5((-!\pyr)-(-!\bOH)=(-!\fur)--(-!\bz)=)}`



EXERCISE Create substructures to simplify the `chemfig` code for the aspirin molecule from tutorial 1 (*HINT* start with benzene).

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



2-Acetoxybenzoic acid (aspirin)