

# CML in ICE

## References

### Wikipedia

[http://en.wikipedia.org/wiki/Chemical\\_Markup\\_Language](http://en.wikipedia.org/wiki/Chemical_Markup_Language)

### CrystalEye

<http://wwmm.ch.cam.ac.uk/crystaleye/summary/index.html>

### CML

<http://wwmm.ch.cam.ac.uk/blogs/cml/>

## What is CML?

According to [Wikipedia](#) CML is:

CML (Chemical Markup Language) is an approach to managing molecular information using tools such as XML and Java. It was the first domain specific implementation based strictly on XML, the most robust and widely used system for precise information management in many areas. It has been developed over more than a decade by Murray-Rust, Rzepa and others and has been tested in many areas and on a variety of machines.

Chemical information is traditionally stored in many different file types which inhibit reuse of the documents. CML uses XML's portability to help CML developers and chemists design interoperable documents. There are a number of tools that can generate, process and view CML documents. Publishers can distribute chemistry within XML documents by using CML.

CML is capable of supporting a wide range of chemical concepts including:

- \* molecules
- \* reactions
- \* spectra and analytical data
- \* computational chemistry
- \* chemical crystallography and materials.

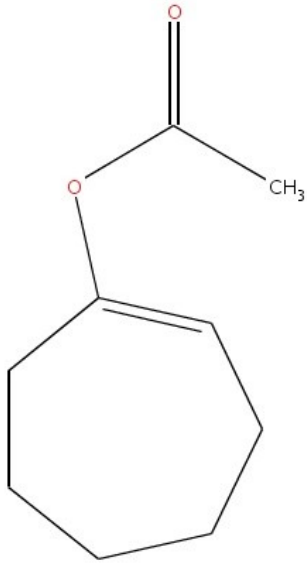
## What do I start with?

Start with a CML file - see an example

Other CML files are available from [Crystaleye](#)

## What can ICE do with CML?

ICE can use the CML to render 3D and 2D images of the chemical structures it describes.

3D image	<p><a href="http://localhost:8000/rep.ice/www/instructions/technical/cml/mol10.htm?embed">http://localhost:8000/rep.ice/www/instructions/technical/cml/mol10.htm?embed</a></p> <p><a href="http://localhost:8000/rep.ice/www/instructions/technical/cml/mol10.htm?embed">http://localhost:8000/rep.ice/www/instructions/technical/cml/mol10.htm?embed</a></p>
2D image	<p><a href="http://localhost:8000/rep.ice/www/instructions/technical/cml/mol10.png?embed">http://localhost:8000/rep.ice/www/instructions/technical/cml/mol10.png?embed</a></p>  <p>The image shows a 2D chemical structure of 1-(cyclohept-1-en-1-yl)acetate. It consists of a seven-membered ring with one double bond. An oxygen atom is attached to the carbon of the double bond, and this oxygen is further bonded to a carbonyl group (C=O) and a methyl group (CH<sub>3</sub>).</p>

## Demo

View our demonstration.

## How-to instructions

1. Save JmolApplet.jar in an ICE folder
2. Save a cml file in the same folder
3. Under the cog-like **options** icon, ensure **Render for ICE** is ticked
4. Suggestions for use:

Embed the resulting html in other ICE documents.

We suggest the use of the 2D image for presentation in the document for PDF renditions with the 3D image visible via a lightbox for web view. eg.

