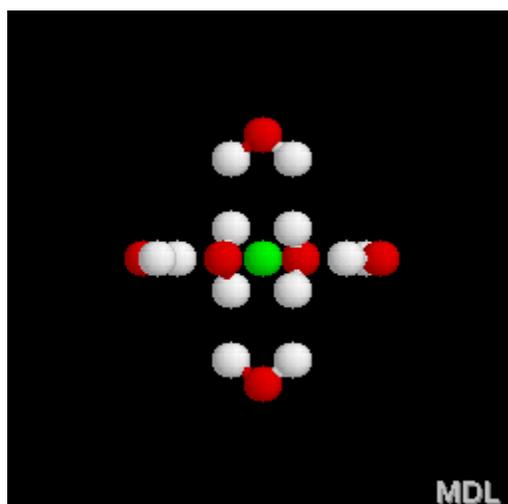# Creating Chime Web Pages in FrontPage:

Interactive Molecular Structures
and
Web-based Learning

hydrated chloride ion

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FrontPage 2000 and 2002 version

Chime is molecular structure rendering software. If you need Chime, it can be downloaded free from http://www.mdl.com/chime. The downloaded file is executable when clicked on and will install itself into your browser. It gives chemists another tool to study molecular structures from the simple to the very complex. For most beginning students, Chime will complement the classical ball and stick model kit used in chemistry. There are a number of file formats that are supported by Chime: .pdb (most common), .mol, and .xyz

Advantages of Chime:

- Freeware – functions as a plug-in for Internet Explorer or Netscape.

- Can be used freestanding in web browser software (file opens directly in browser in the wireframe display mode) or Chime images can be incorporated into web pages using FrontPage or Netscape Composer.

- Interactive – molecular structure can be positioned by using the mouse; measurements, such as bond distances, bond angles, and torsion angle, can be accomplished. You can zoom into large structures to view segments.

- Menu-driven using the mouse and right click or using buttons and script writing.

- Provides multiple representations of molecules – wireframe, ball and stick, and space-filled modes. For proteins and nucleotides, cartoons (ribbons for helices and sheets) can be generated for examining units or bulk structure.

- Can display electrostatic potentials maps – these colored surfaces indicate the distribution of charge on a molecule. They are very useful when considering molecular polarity for determining the behavior of physical properties and how a molecule will be attacked in a reaction mechanism.

- Allow animations – reaction mechanisms or molecular vibrations can be produced. An animated Chime file will be in the .xyz format.

The application of Chime in webpages can be found on many websites. For large complicated biological molecules, Chime is an elegant tool for structure examination. For example, see Duane Sears' Instructional Biochemistry site at http://tutor.lscf.ucsb.edu/instdev/sears/biochemistry.

Creating a webpage in FrontPage
A web page usually requires a number of embedded files such as Chime images and other graphics. For efficiency, create a folder in which you will save the FrontPage file and place the Chime files that you are going to use in the FrontPage document into this folder.
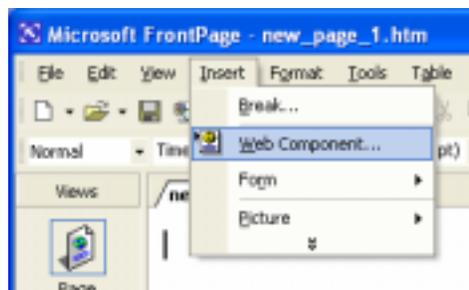
Inserting a Chime file into a FrontPage 2000 document
The Chime file is considered a plug-in in FrontPage. Go to "Insert" on the menu bar, select "Advanced", and then select "Plug-In…"
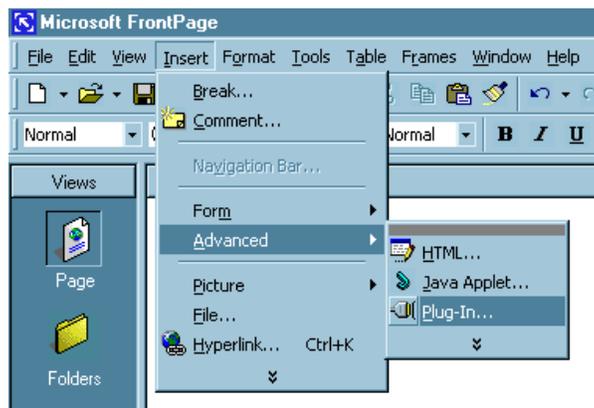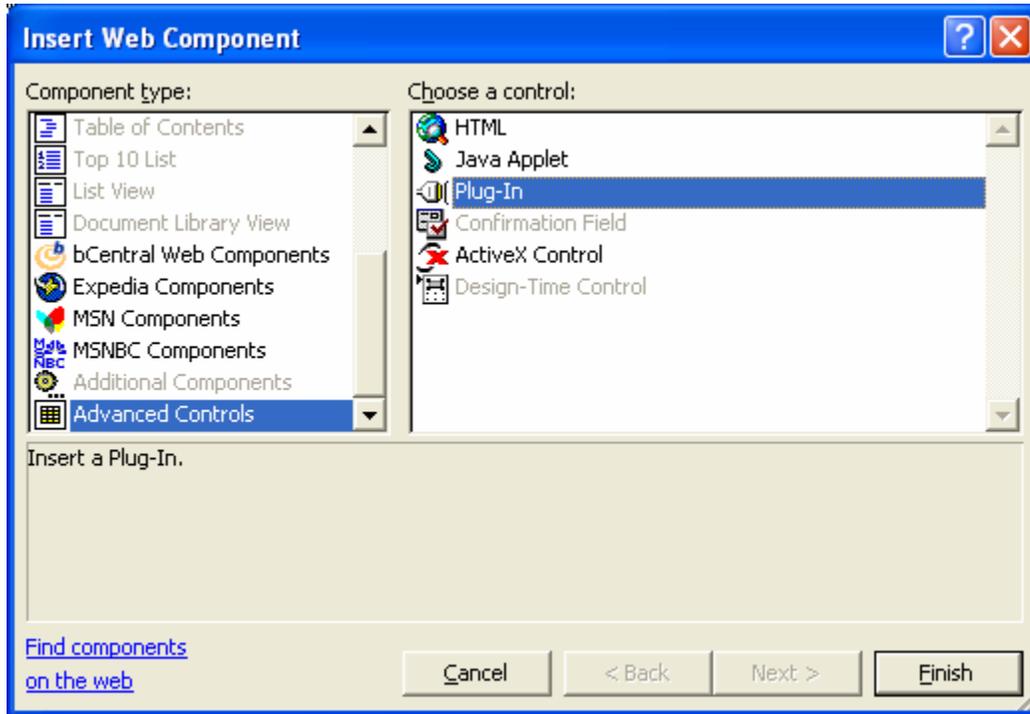

Inserting a Chime file into a FrontPage 2002 document
Go to "Insert" on the menu bar and select "Web Component…"

The "Insert Web Component" box will appear. On the "Component type" list to the left, scroll to the bottom of this list to find "Advanced Controls", and click on it. From the "Choose a control" list on the right, select "Plug-In" and then press the Finish button.


Handling the Plug-In
After you select plug-in in either version, the "Plug-in Properties" box should appear. Select the "Browse…" button and locate your file and select it. Your file name will then appear in the "Data source:" box. Set the 'Height" and "Width" each to 250, and then click OK.
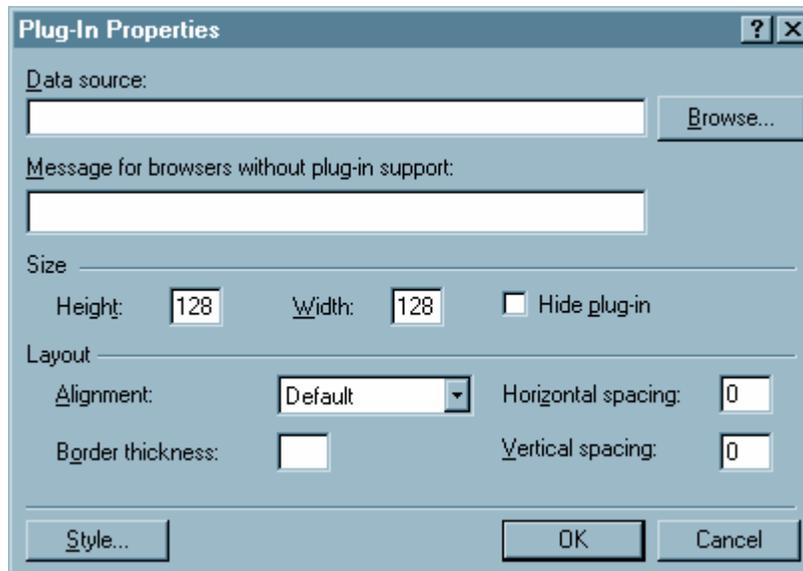
You should see the screen shown below, indicating the Chime file has been placed into the document. Since we increased the size of the image, the file name also appears.
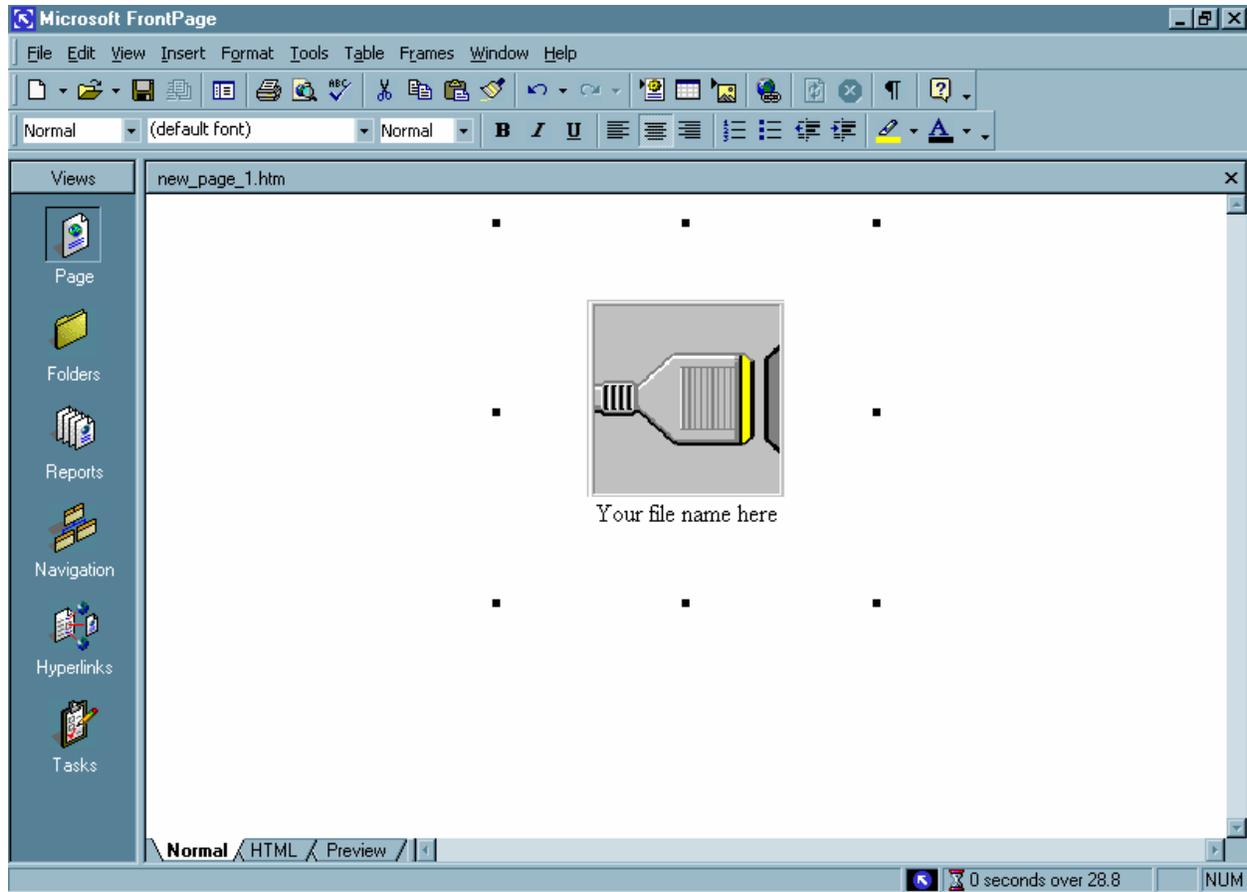
If you right click within the area of the black squares of the plug-in, a menu will appear. Select "Plug-In Properties..." to resize the Chime image.

To place another Chime image into the document, you can copy the first one and then paste. Right click on the new or second plug-in and select "Plug-In Properties" and browse to change the file name. This method also copies any added embedded tags (see next section).

You can place a number of Chime images next to each other depending on the size you select for them.

Once you have the Chime images in place, if you click on the Preview tab at the bottom left of FrontPage, you will see the Chime image. The default for any Chime image is the Wireframe display. To change this, you need to add some HTML code.

A better preview of the page in your browser can be generated under "File" on the menu bar and then select "Preview in Browser…" This can be done after you have saved the FrontPage file.

Writing HTML code
We are adding what are called embedded tags to the HTML code.

Find the line of code shown below by clicking on the HTML tab:

```
<embed width="250" height="250" src="NH3.pdb">
```

Notice you can change the size here and identify the Chime file name (NH3.pdb).

Add the display3d= "ball&stick" (do not worry about the color, FrontPage will take care of this).

```
<embed width="250" height="250" src="NH3.pdb" display3d= "ball&stick">
```

For space-filled molecules-

```
<embed width="250" height="250" src="NH3.pdb" display3d= "spacefill">
```

If you want the molecule to rotate around add: `startspin= "yes"`

If you want the Chime image to come up as the electrostatic potential map, you need to add the following after removing any display3d tag:

```
script="
  surface smoothing white
  list smoothing transparent false
  calc charges true
  set MEP mode rasmol
  set MEP mode true
  color list smoothing mep rasmol
  selectall
  "
```

If you want the map to be transparent change this line to:

```
    list smoothing transparent true
```

Some Chime files are animations. They will always be of the xyz format (.xyz). To get these files to play constantly in a webpage, you must add three embedded tags.

```
animfps= 40 startanim= true animmode= loop
```

The animfps controls the speed in frames per second and can be adjusted.

The easiest way to learn to write HTML code is to view the code on a webpage where you see something you like. On a webpage, right click and select view source on the menu that appears (make sure the cursor is NOT on the Chime image; place it on text). You may need to search around to find the embedded Chime file and the code example you want.

For more explanation on embedded tags, see the MDL site at http://www.mdl.com/chime/chimeembed.html.

<u>Writing HTML code for the use of interactive buttons</u>
For angle measurement:
within the embedded Chime file add (this directs the button to this Chime file)

```
name= "model1"
```

then follow this with

```
<embed
      type= "application/x-spt"
      width= 20
      height= 20
      button= push
      target= "model1"
      script= "set picking angle"
>
```

which creates the button and targets it to the Chime file.

For electrostatic potential map:
within embedded Chime file add

```
name= "model1"
```

then follow this with

```
<embed
     type= "application/x-spt"
     target= "model1"
     button= "push"
     width= "20"
     height= "20"
     script= "select *; surface testSurf MEP rasmol"
>
```

For the use of buttons, each Chime file must have a unique name and the button used must have the same unique target. For multiple buttons, copy and paste and just change the target name as you go.

For further explanation on the use of buttons, see Molecules in Cyberspace: Tutorial for Embedding Chime Images into Web Pages at http://www.chem.uwec.edu/EmbeddingChimes/index.html.

Finding Chime structures
A good starting source of 400 Chime molecules is the Molecular Library from Cabrillo College at http://c4.cabrillo.cc.ca.us. The library is downloaded as a zipped file.

Finding structures on the Internet can be accomplished by a search using Google (http://www.google.com), where the chemical formula or name followed by the word chime is entered such as NO2 chime or aspirin chime.

You can save a Chime image from a website. Right click on the image and select "File" and then "Save File As…" If you select "Edit" and then "Copy", you can paste a *static* image into Word documents or PowerPoint slides.

Beware that some structures may have the correct atomic connectivity but incorrect bond lengths and bond angles.

Designing your own activity
Pick a pair of molecules or a small group of related molecules and create a web page. Design the page as a series of questions that explore the molecules by measuring bond distances and/or bond angles or explore polarity using the electrostatic potential map.

Examples of short guided-inquiry activities can be found at
http://academic.pgcc.edu/~ssinex/struc_bond/structure_and_bonding.htm.

See the Chime Guide at http://academic.pgcc.edu/psc/chime_guide.html for help
and designing your instructions for your students.

Here are some examples to build a short activity around.

▶   Compare the bond lengths in single and double oxygen bonds and then
measure ozone.

▶   Does adding iodine to CH_4 to make CH_3I change the bond angles? If so,
why?

▶   Compare the geometries of Cl_2O, ClO_2, and Cl_2O_7 or SO_2 and SO_3.

▶   Are all C-H bond lengths equal? Compare in ethane, ethene, and ethyne.

▶   Compare the nitrate ion with nitric acid. (nitrite ion and nitrous acid)

▶   How do the boiling points of CH_4, CH_3OH, and CH_3SH compare and why?

Importing other images
Other images can be added into FrontPage by going to "Insert", and then select
"Picture". From here you can add clip art, images from files, and videos. Animated
gif files are added as pictures from files. They are only animated in the preview
mode or when opened in the browser.

Graphs from Excel can be copied in Excel and then pasted directly into FrontPage.
You cannot modify an Excel graph in FrontPage. When you save the FrontPage file,
it will collect the images including stuff from the clipboard and save it with your
FrontPage file in your folder.

Adding hyperlinks
First open the website you want to link to in your browser. Back in FrontPage, go
to "Insert", select "Hyperlink…" and when the "Insert Hyperlink" box appears, click
on your web browser and bring up the site you want. When you return to
FrontPage, the URL will be in the address box. A good way to avoid typing errors!

Internet Sources of Chime Structures

Structures	Websites
A variety of inorganic and organic structures	http://www.wellesley.edu/Chemistry/Flick/molecules/newlist.html
	http://people.ouc.bc.ca/woodcock/molecule/molecule.html
Biochemical molecules	http://info.bio.cmu.edu/Courses/BiochemMols/BCMolecules.html
	http://www.clunet.edu/BioDev/omm/gallery.htm#top
Minerals and crystalline solids	http://www.soils.wisc.edu/virtual_museum/displays.html
	http://www.molecules.org/elements.html
Vibrations in molecules	http://www.chem.purdue.edu/gchelp/vibs/
	http://www2d.biglobe.ne.jp/~chem_env/mva/indexE.html
Animations of reaction mechanisms	http://www.cmbi.kun.nl/wetche/organic/

Note: With many crystalline structures you may see nothing in wireframe display mode. Hence, change the display to ball and stick!