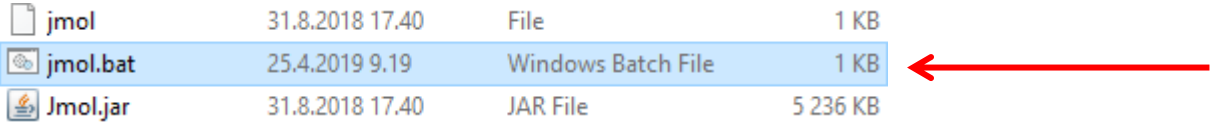
Jmol installation and basic use

Installation of Jmol (1)

- Jmol is a versatile program for visualization and manipulation of molecules and crystal structures
- It runs on Windows, macOS, and Linux
- We will be using Jmol throughout the exercise sessions
- Let’s first ”install” it in on your computer (instructions for Windows 10):

Installation of Jmol (2)

1. MyCourses -> Solid State Chemistry -> Software -> Jmol
2. Download the **zip file** on the computer (works on Windows/macOS/Linux)
3. Save the file anywhere you like (even Desktop is fine, that's easy to find)
4. Extract the zip file (for example by right-clicking and choosing **Extract All…**)
   - You will get a folder ***jmol-x.y.z***, where *x.y.z* is the version
   - If you start Jmol from the zip file without extracting it, Jmol will not work right!
5. Jmol is now "installed"
6. Go to the folder ***jmol-x.y.z*** and double-click ***jmol.bat*** to start Jmol
   - If you do not see the file extensions, double-click the file whose type is "Windows Batch File" (small gears in a window):



   - If ***jmol.bat*** does not work, try double-clicking ***Jmol.jar***
   - If Jmol does not start, you may need to install the Java Runtime Environment (see the next slide)

Java Runtime Environment (JRE)

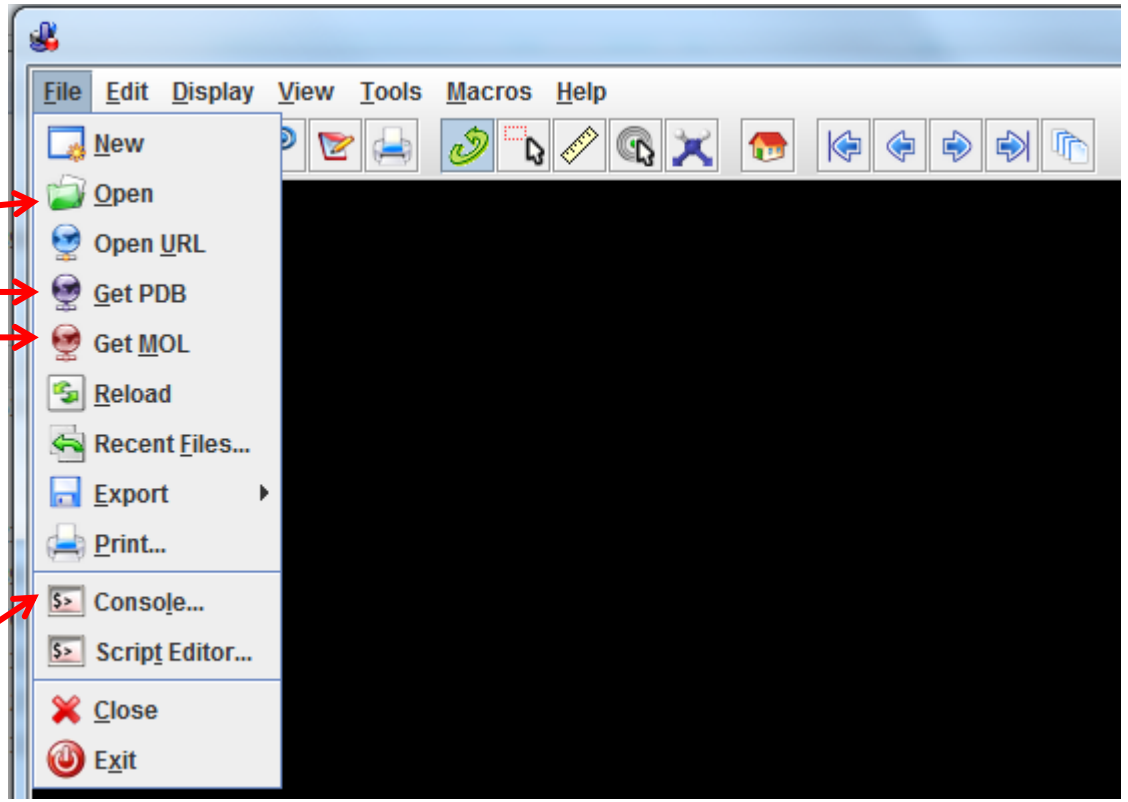
- **Only read this slide if**
  - You are using your own computer (Windows, Mac, or Linux)
  - Jmol does not start when you double-click ***jmol.bat*** or ***Jmol.jar***
- **If you are working in an Aalto Computer class, please skip this slide!**

- Go to https://www.java.com/en/download/ and click ”Agree and Start Free Download”
- Install the downloaded package
- If Jmol still does not start after this, please try restarting your (Windows) computer

- Additional information:
  - You do not necessarily have to download the proprietary JRE from Oracle
  - There is also an open source alternative available at https://jdk.java.net/15/
  - It may require bit more tweaking to get it working

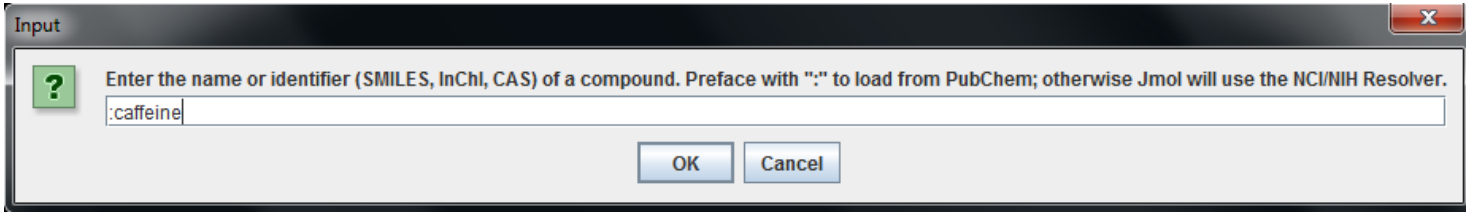
File menu

- We will obtain crystal structures as CIF files from various databases
- They can be opened via File -> Open
- ”Get MOL” and ”Get PDB” offer interfaces to PubChem and PDB databases. But the menu items do not always work and we will use Console instead.
- ”Console...” opens up a console for typing text commands. We will use this one a lot



Loading a molecule from PubChem (1)

- Choose ***File*** -> ***Get MOL***. Enter ***:caffeine*** into the input box and click OK

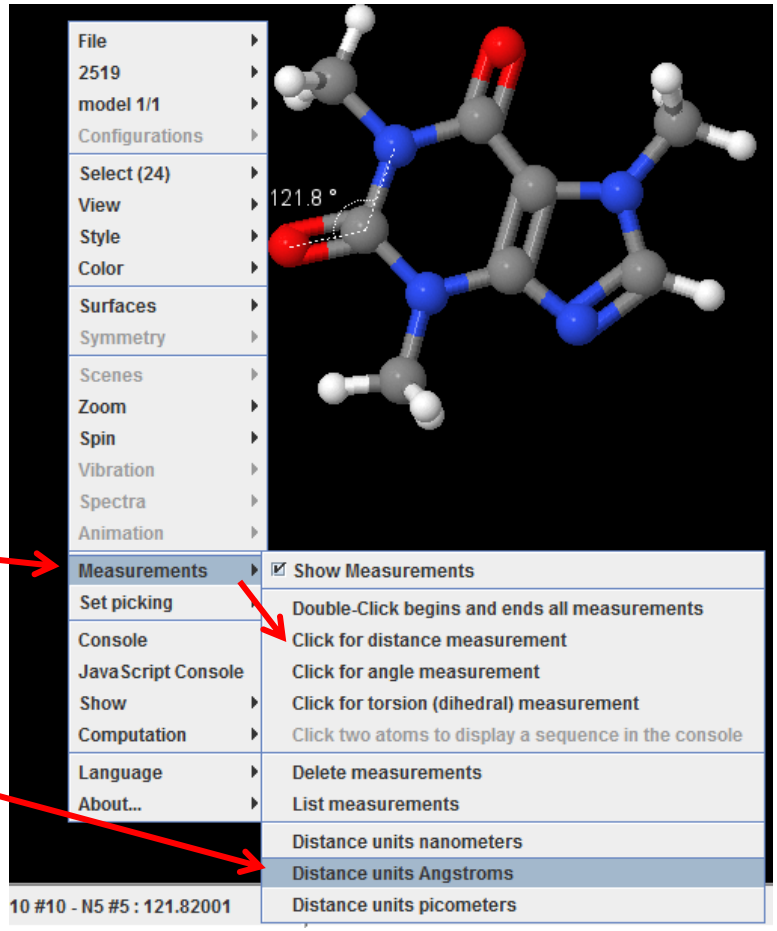


- If the Get MOL menu item does nothing or gives an error, use the Console:
  - Open ***File -> Console***
  - Type into the console **load :caffeine**
  - There must be a space between load and :, but not between : and caffeine

- Jmol will load the molecule from PubChem
- https://pubchem.ncbi.nlm.nih.gov/
- Over 109 000 000 compounds (2021-01-12)

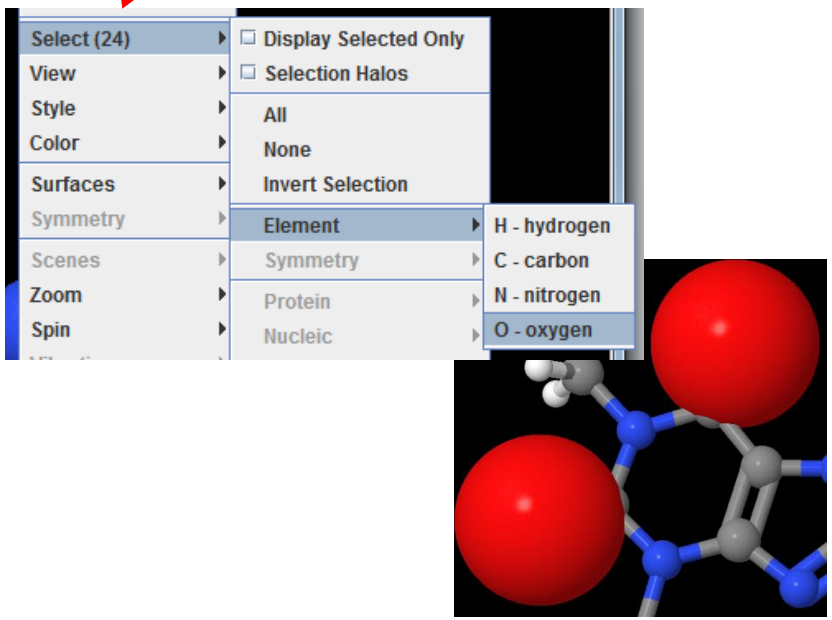
Loading a molecule from PubChem (2)

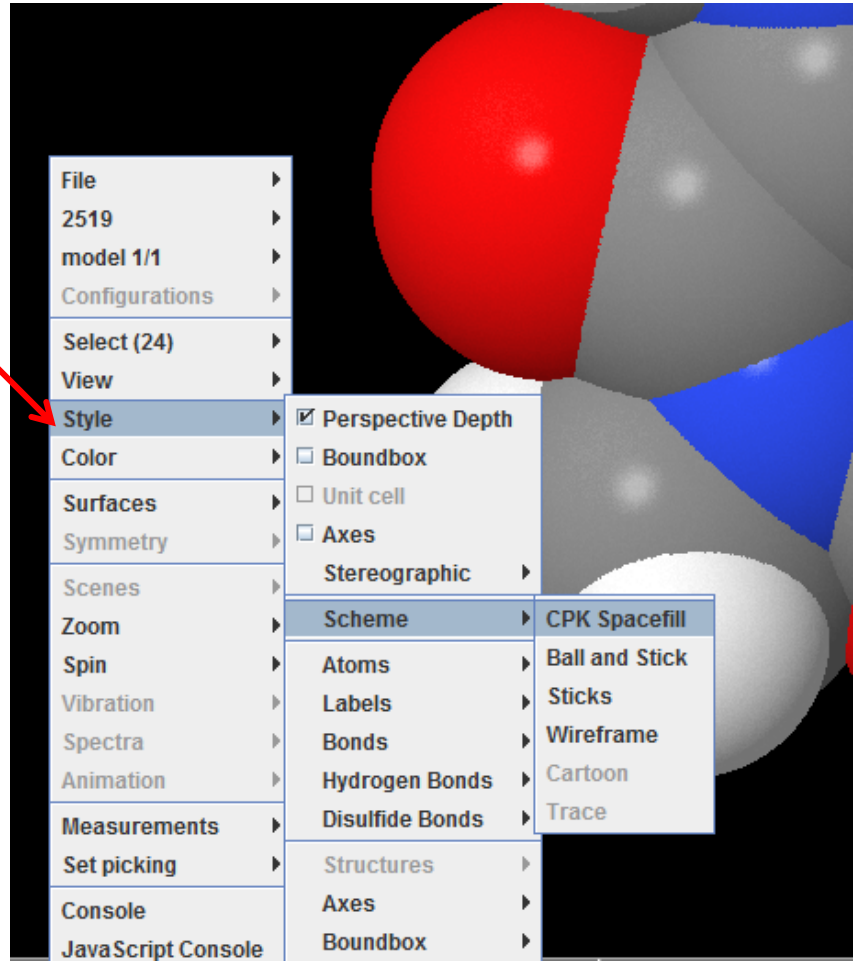
- After the caffeine molecule has loaded, try moving it:
  - Hold left mouse button to ***rotate***
  - Use mouse wheel to ***zoom***
  - Ctrl + right mouse button to ***translate***
  - Shift + left button:
    - Mouse left/right: rotate in plane
    - Mouse up/down: zoom
- **Right-click** the window to get a menu
  - Try measuring some distances and angles
  - Set Distance units to Angstroms before measurements



Controls

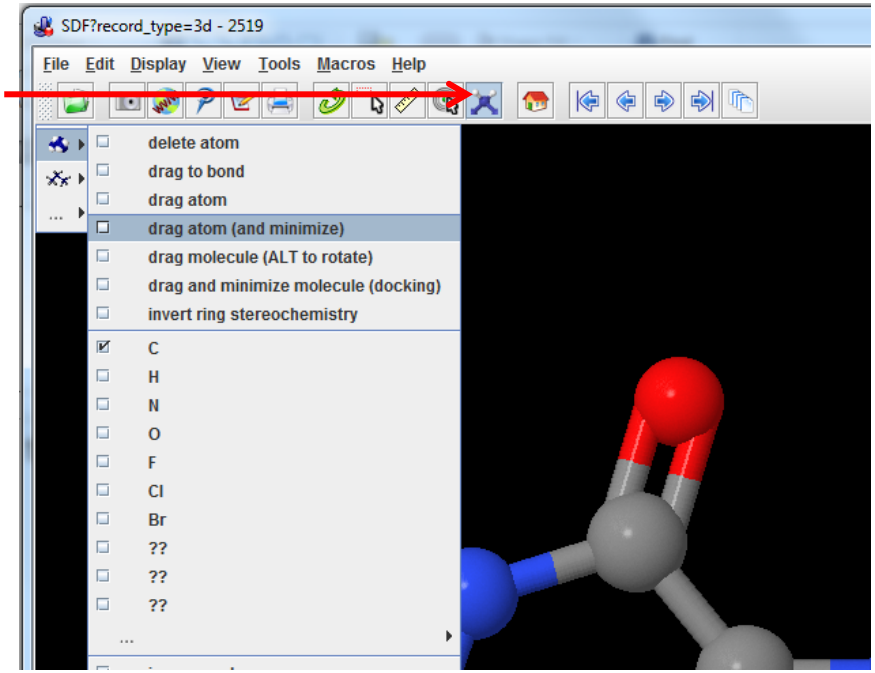
- Try changing the display settings
  - CPK spacefill -> sometimes very useful for understanding e.g. steric constraints
  - You can also select just some atoms and then change their properties





Model kit

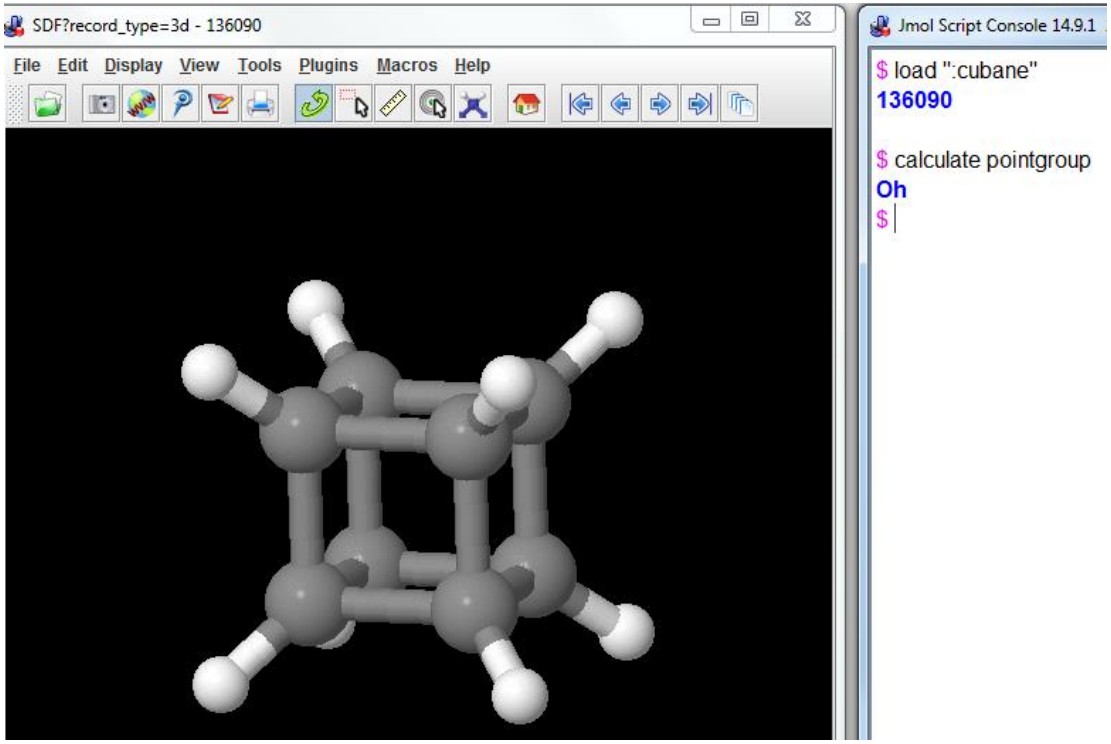
- Jmol can also be used to build molecules (it is not an ideal solution for that)
- You can try the model kit and for example modify the caffeine molecule
- Warning! The ***Drag atom (and minimize)*** tool can be very addictive! (choose it, start dragging an atom and see what happens when you release the mouse button)



- Try to load few more molecules with "Get MOL" or Console -> load :molecule
  - :aspirin, :ibuprofen, :dodecahedrane, :tnt, your favorite molecule, …
- Some additional commands that may be helpful (but not used on this course):
  - To export the XYZ coordinates of any molecule, first open ***File -> Console***
  - To print out the XYZ coordinates (for copy-pasting), execute ***write xyz***
  - ***write filename.xyz*** writes directly to a file (in the Jmol folder)

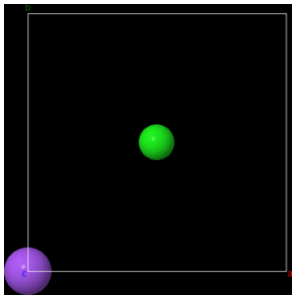
Point group symmetries

- One more useful feature in Jmol is the point group symmetry detection
- open ***File -> Console***
- Execute **load :cubane** to directly load cubane from PubChem
- Execute **calculate pointgroup** to determine the point group symmetry -> **Oh**!
- For more information, execute **help calculate** (*e.g.* to make the search less strict)



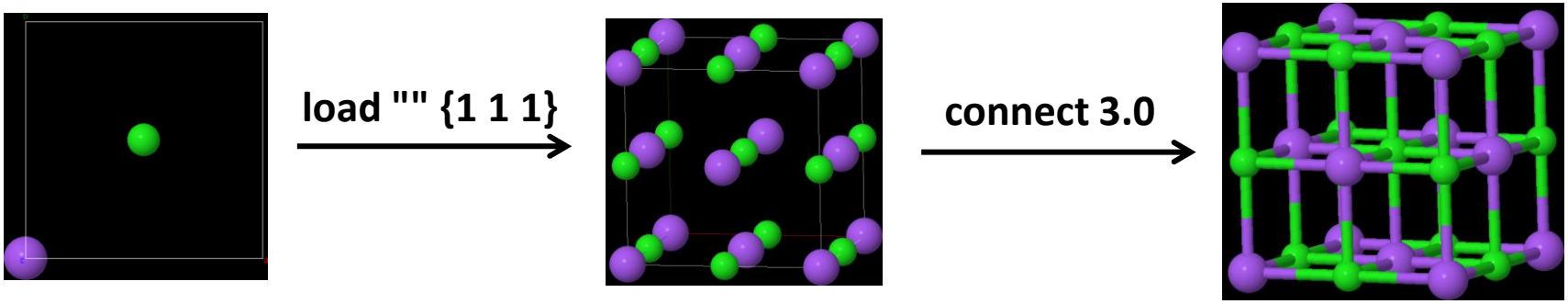
Loading a crystal structure from Crystallography Open Database (COD)

- COD (http://www.crystallography.net/) is an open access crystal structure database
- Using COD from Jmol is very easy:
  - First, find out the COD ID of the crystal structure via the COD web interface
  - Let's use a NaCl structure as an example (COD ID **1000041)**
  - In Jmol, open ***File -> Console***
  - Type into the console: **load =cod/1000041**
  - There must be one **space** between **load** and **=**
- The structure should load right away!
- This is easier than saving a CIF from COD and opening it in Jmol (File -> Open)
- The structure probably first looks like this:
- Let's modify the appearance next

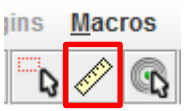


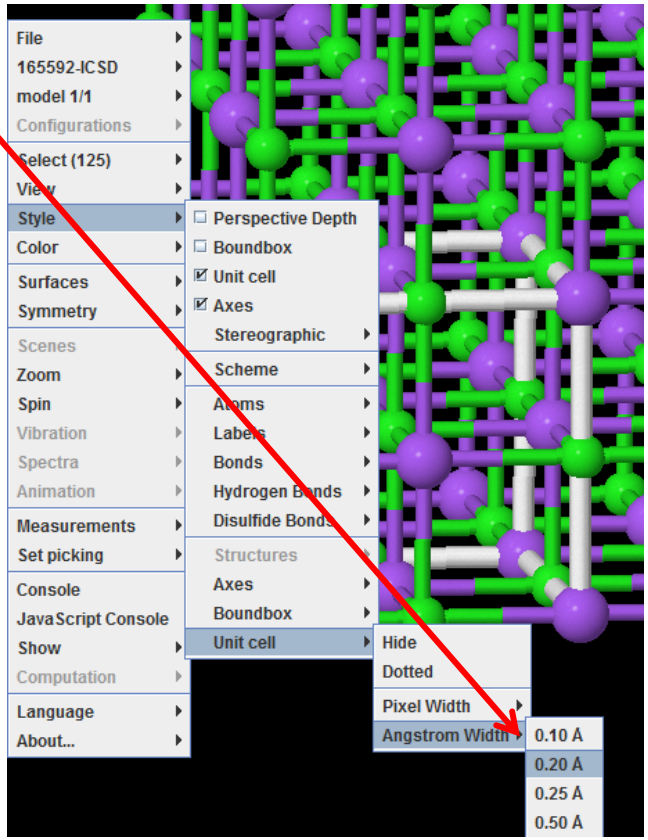
Tuning crystal structure appearance

- To show the unit cell properly, type into the console: **load "" {1 1 1}**
  - "" = two quotes. Note that **{1 1 1}** has spaces between the numbers!
  - **load ""** means “reload the current structure”
  - load "" {a b c} can be used to draw any kind of *supercell*, e.g. **load "" {4 2 2}**
  - The other way is to right-click -> Symmetry -> Reload {1 1 1}
- Draw bonds with **connect 3.0** (connects all atoms with distance < 3.0 Å)
  - More generally: **connect 2.5 3.0 {_Na} {_Cl}** (min, max, from_atom, to_atom)
  - Execute **help connect** if you want to have more information



Further tips for crystal structures

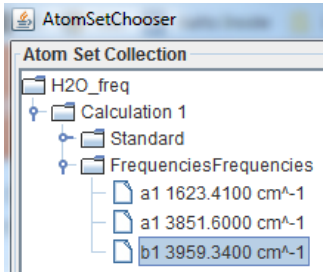
- Load a larger supercell by entering the following:
  - **load "" {2 2 2}**
  - **connect 3.0**
- To see unit cell edges better, increase the edge width:
- ***Symmetry -> HM:Fm-3m*** can be used to visualize space group symmetry operations! Try e.g. C_3 rotation **3** or mirror plane **23**
- Distance measurements work similarly to molecules
  - Right-click -> Measurements
  - You can also use the measurement tool in the main menu bar: 



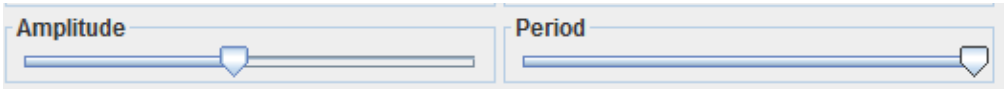
Advanced Jmol topics (starting from Lecture 8)

Visualizing vibrations with Jmol

- Vibrational modes can be visualized in Jmol
  - This enables us to interpret IR/Raman spectra
  - … after someone has first run the quantum chemical spectrum calculation
- Download Materials -> Data files for lectures -> Lecture 8 -> **H2O_freq.log**
- The file includes the vibrational modes of H_2O
- Open the file in Jmol (Jmol first loads the structure of H_2O)
- To visualize the vibrational modes, go to **Tools** -> **AtomSetChooser**.
- The vibrational frequencies are under Calculation 1 -> Frequencies ->
- Choose a mode and click "Play" button under "Vibration":



- "Amplitude" slider can be used to increase the amplitude
- Period slider can be used to make the vibration slower of faster



- **Important**: you typically need much larger amplitude for visualization :
  - Right-click the main screen -> "Vibration" -> "*2" (can be done several times)

Figures: AJK