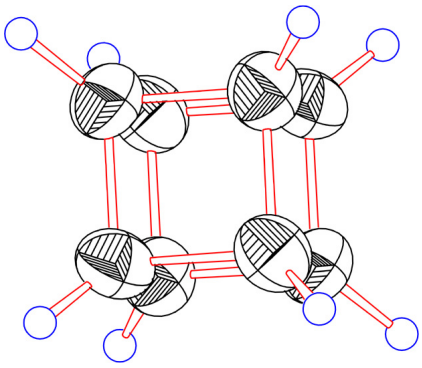
iORTEP

A Crystallographic Plotting Program

Fortran version by Carroll K. Johnson, 1976
Interactive version by G. C. Lisensky, 2003-2022

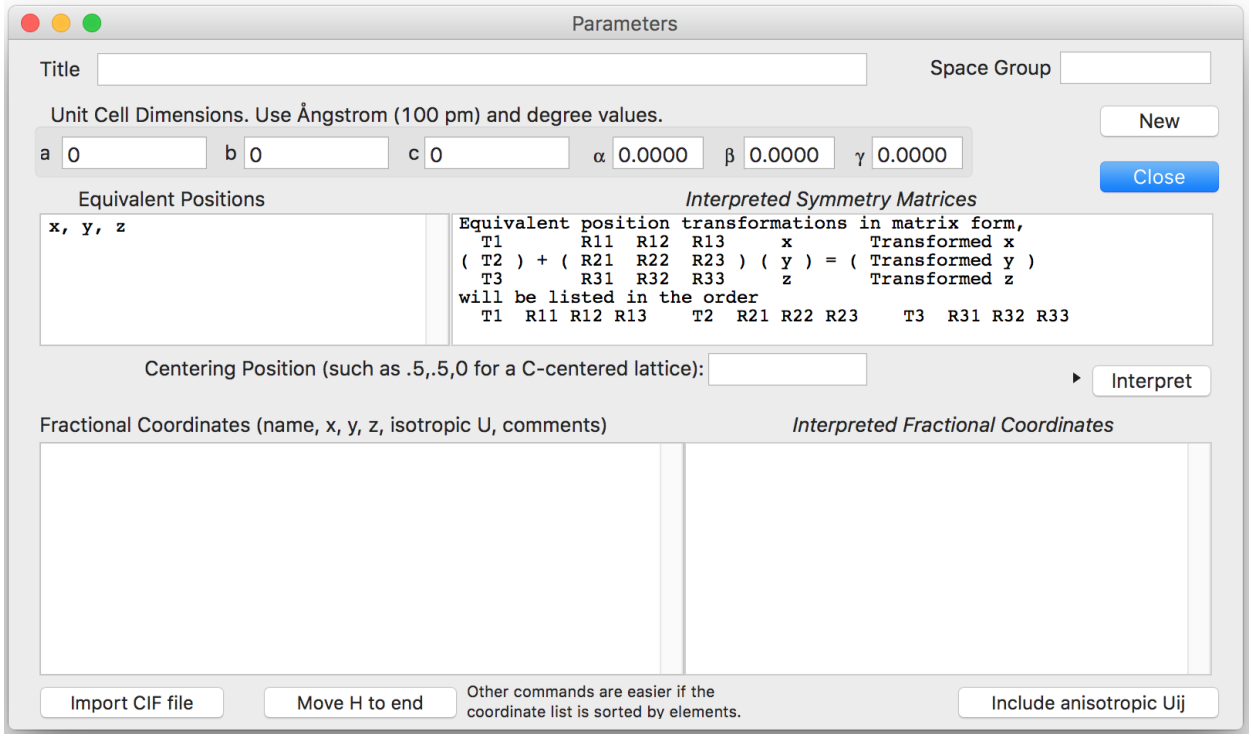


To plot a crystal structure you need to enter values for
- the unit cell dimensions (axes in Å, angles in degrees),
- the space group symmetry (equivalent positions and centering),
- a unique name, fractional coordinates and thermal parameters for each atom.

Example. Consider the structure of cubane. C_8H_8 crystallizes in space group $R\bar{3}$ with unit cell dimensions 5.34 Å and 72.26°. The fractional coordinates are:

Atom	*x*	*y*	*z*
C1	–.18711	0.19519	0.10706
C2	0.11546	0.11546	0.11546
H1	–.32460	0.34680	0.18480
H2	0.21000	0.21000	0.21000

Parameters to enter data.



- You can use any text you want for title and space group, but actual names are helpful.
- Press TAB to go from one entry to the next. Click **Close** when all values are entered.
- Centering positions will be added to the equivalent positions when you click **Interpret**.
- If you paste text, use **Interpret** to see if extra characters are correctly removed.
- Remember to **Save** you work occasionally so you can use **Load** to continue your work.

Individual atoms are referred to by an ATOM DESIGNATOR CODE:
• The last two digits refer to the symmetry equivalent positions in the order entered.
• The next three digits refer to translations along the *abc* directions, each digit referring to one axis direction. Examples:
    555 is no movement,
    655 is one unit cell translation along *a*,
    554 is minus one unit cell translation along *c*, and
    656 is one unit cell translation along both *a* and *c*.
• The remaining digit(s) refer to the atoms in the order entered.

Thus 1256504 (think of this as 12 565 04) is the twelfth atom in the original atom list operated on the fourth symmetry element in the equivalent positions list, followed by translation of one unit cell along *b*.

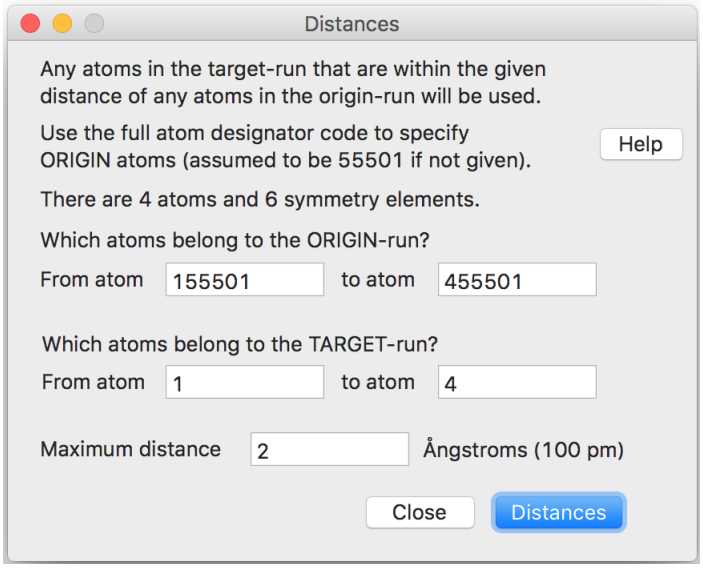
Sets of atoms are described by atom RUNS.
For example, from 1 to 3 indicates 155501, 255501, 355501.
From 154501 to 365503 thus indicates

154501, 254501, 354501,	155501, 255501, 355501,	165501, 265501, 365501,
154502, 254502, 354502,	155502, 255502, 355502,	165502, 265502, 365502,
154503, 254503, 354503,	155503, 255503, 355503,	165503, 265503, 365503.

What are the bond distances and angles in the molecule?

Distances

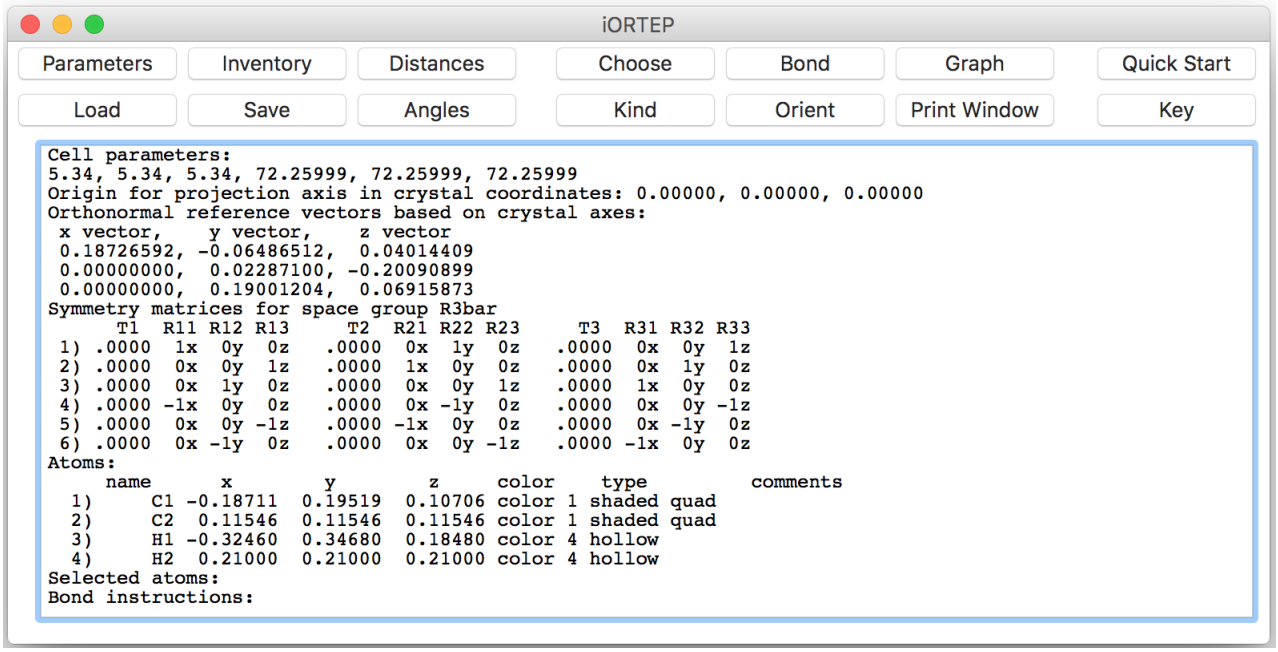
Angles is similar (but use distances first to make sure you are not finding too many values.)



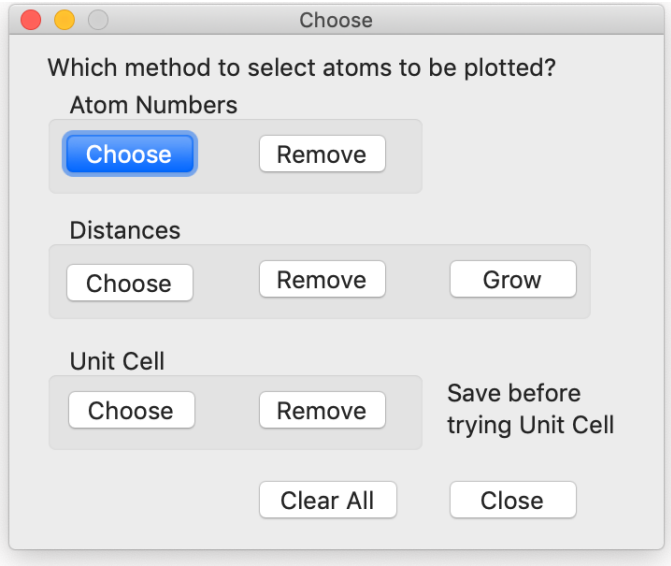

```
                CODE        x         y         z
Distance from( 155501) -0.1871,  0.1952,  0.1071 to  1 thru 4
    C1   H1   ( 355501) -0.3246,  0.3468,  0.1848 is  1.0118 Å (100 pm)
    C1   C1   ( 155505) -0.1071,  0.1871, -0.1952 is  1.5493 Å (100 pm)
    C1   C1   ( 155506) -0.1952, -0.1071,  0.1871 is  1.5493 Å (100 pm)
    C1   C2   ( 255501)  0.1155,  0.1155,  0.1155 is  1.5515 Å (100 pm)

                CODE        x         y         z
Distance from( 255501)  0.1155,  0.1155,  0.1155 to  1 thru 4
    C2   H2   ( 455501)  0.2100,  0.2100,  0.2100 is  1.1093 Å (100 pm)
    C2   C1   ( 155502)  0.1071, -0.1871,  0.1952 is  1.5515 Å (100 pm)
    C2   C1   ( 155503)  0.1952,  0.1071, -0.1871 is  1.5515 Å (100 pm)
    C2   C1   ( 155501) -0.1871,  0.1952,  0.1071 is  1.5515 Å (100 pm)
```

Print Window will print the values you find.

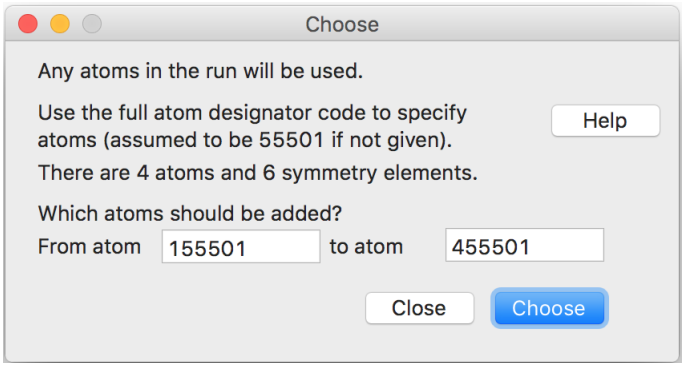
Load to resume your work later. (Use **Inventory** to see this page again.)



Choose to select the atoms to be plotted. If no atoms are selected then none will be plotted.



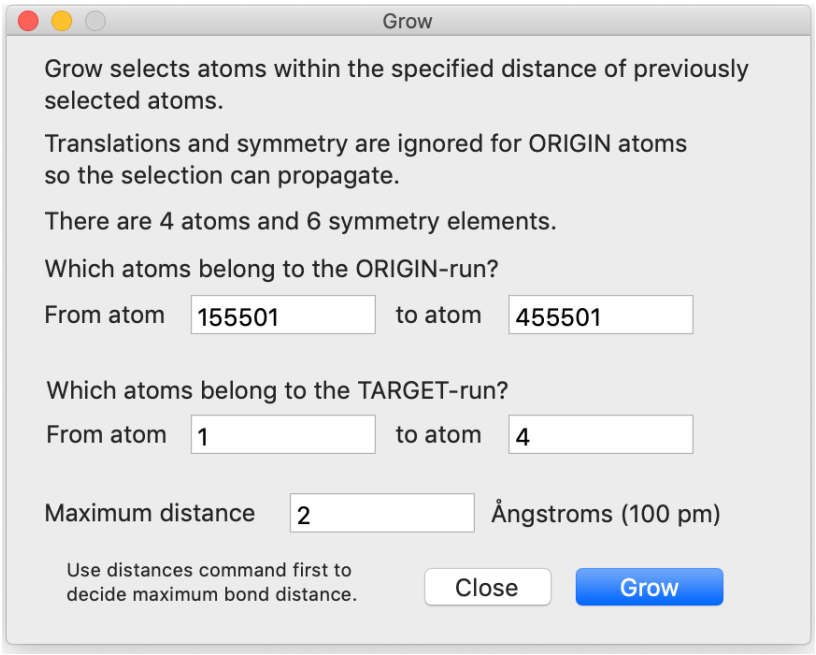
Choose (Atom numbers)




```
Selected atoms:
 155501, 255501, 355501, 455501
```

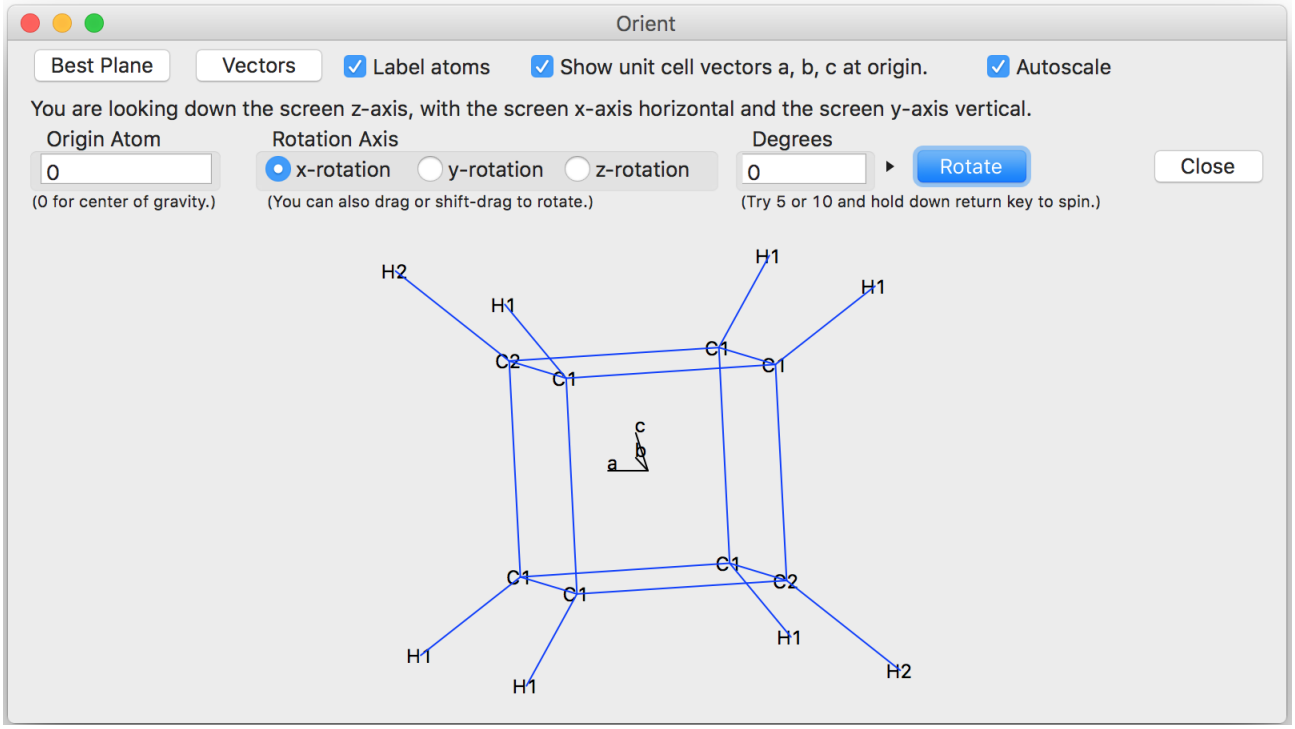
Save frequently so you can revert back if something unexpected happens. ORTEP parameter files are very small.

Choose (Grow) to find the rest of the molecule. The distance must be short enough to exclude additional molecules. (Not recommended for polymers!)




```
Selected atoms:
 155501, 255501, 355501, 455501, 155505, 155506, 155502, 155503
 255504, 355505, 355506, 355502, 155504, 355503, 455504, 355504
```

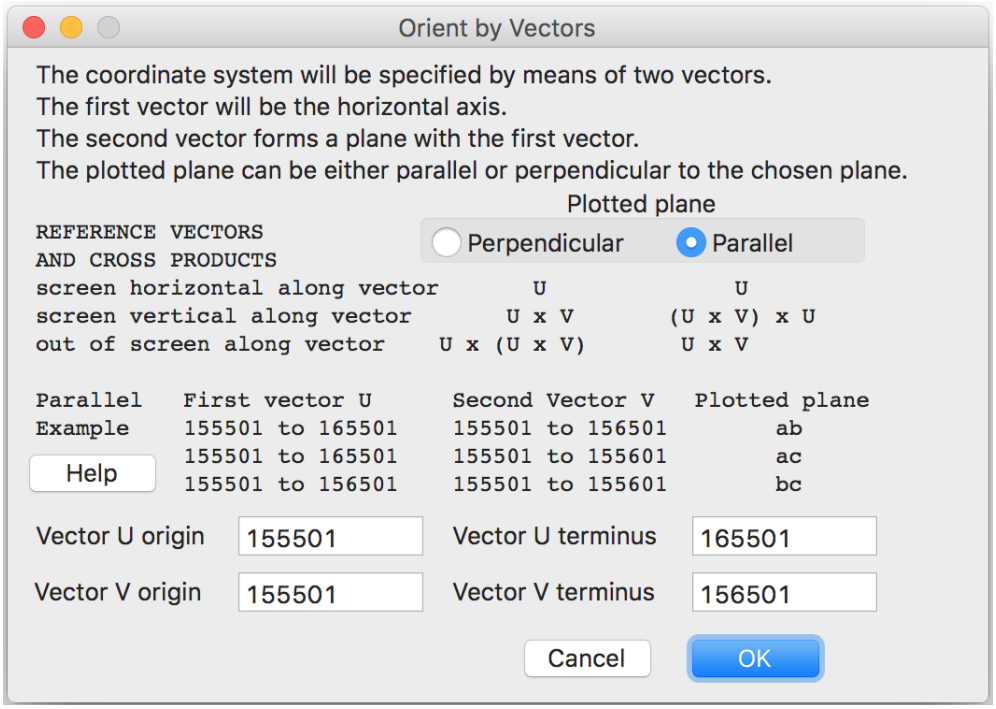
Orient (Best Plane) makes the view plane the least squares best plane for the molecule. This often provides an excellent orientation.
Orient (Rotate) is useful for adjusting the orientation. Try 5 or 10 degrees and repeatedly press RETURN for small adjustments.



The origin atom is the in-plane center of the plot. 0 is usually the best choice but you might want to rotate around a central metal atom instead.

The orientation is saved in the ORTEP file; save a file for each view you wish to keep.

Orient (Vectors) to specify the exact view.

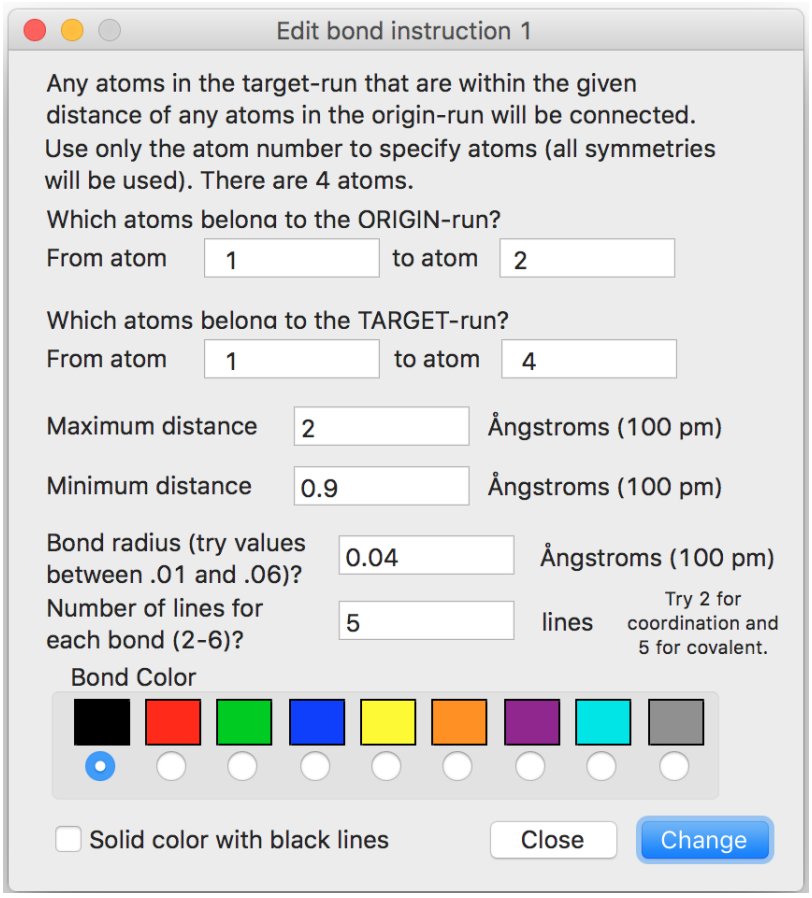


Bond defines the bonds in the molecule. You should previously have used the **Distances** command so you have some idea of what distances to call a bond.

You will normally need to have different commands to specify distances for metals and ligands, for carbons, and for hydrogen.

It is often useful to indicate coordination bonds by using a 2-line bond and covalent bonds by using more lines.

If solid color is selected, the background of the bond will be the chosen color; if solid color is not selected the lines themselves will be the chosen color.



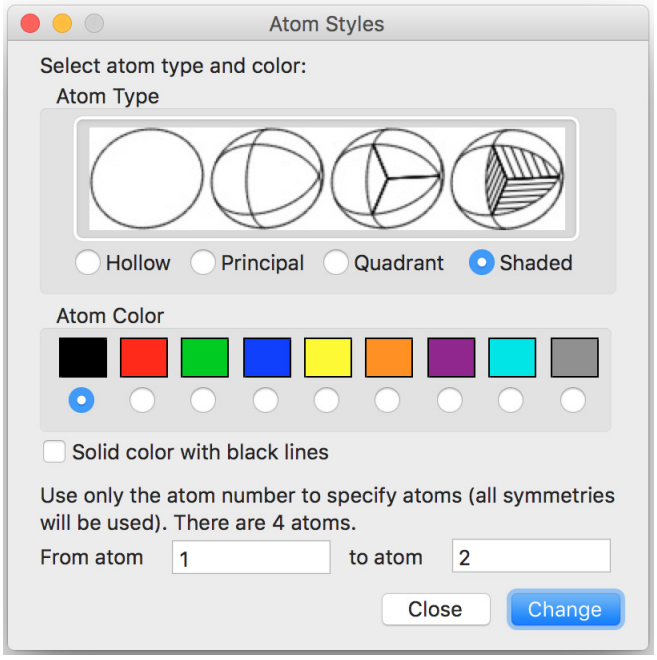

```
Bond instructions
1) From atoms  1 thru  2 to  1 thru  4 within  0.9 thru  2.0 Å,
   connected with 0.04 Å radius bond of 6 lines of color 2.
```

Kind selects the atom types and colors.

To show the ellipses you need to enter anisotropic thermal parameters on the parameter pages.

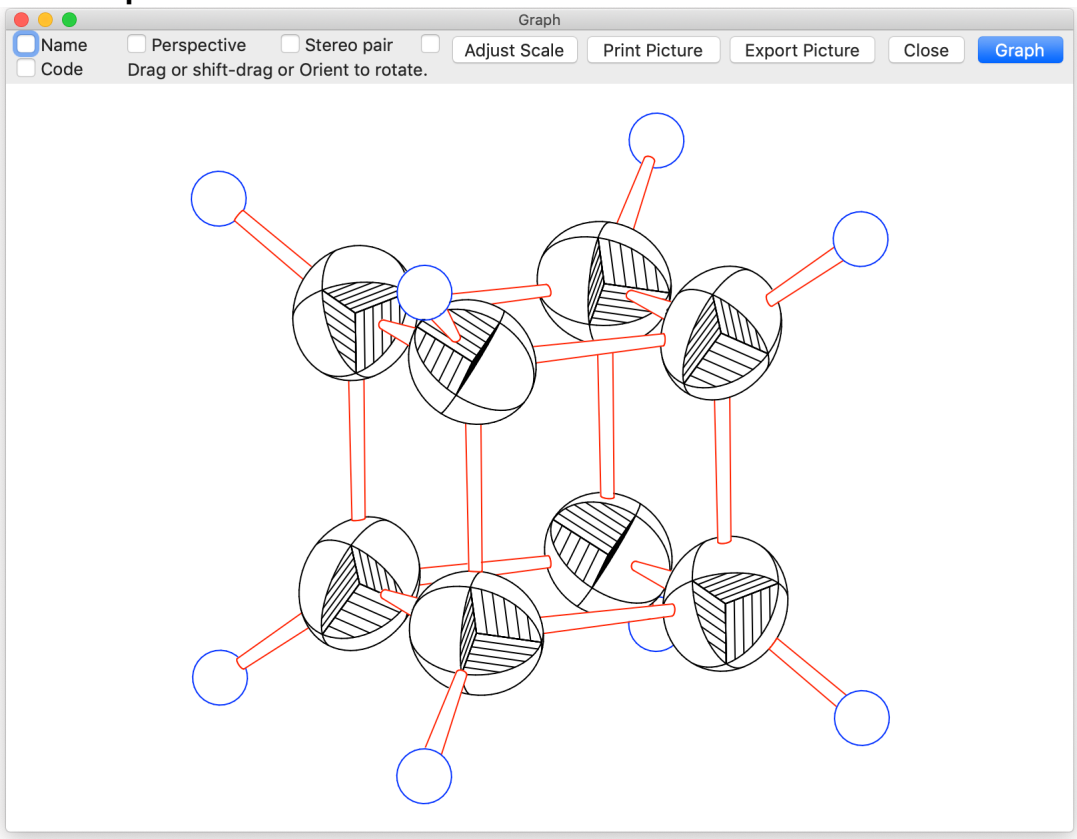
If solid color is selected, the body of the atom will be the chosen color; if solid color is not selected the lines themselves will be the chosen color.

You should make every element a different color or style. **Key** can be used to provide a legend to go with **Graph**.

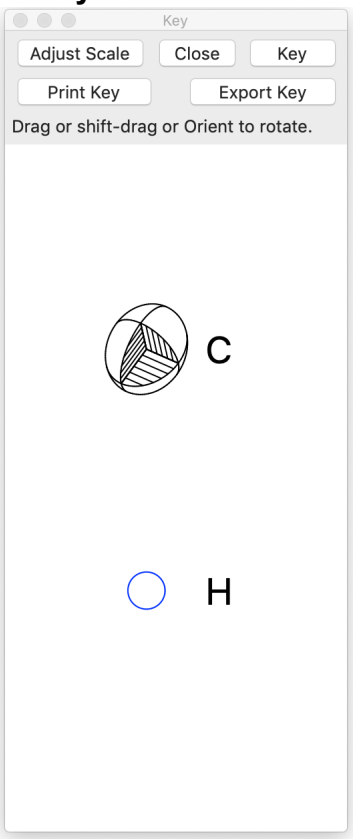



```
Atoms:
    name        x         y         z     color    type          comments
 1)     C1  -0.18711   0.19519   0.10706 color 1 shaded quad
 2)     C2   0.11546   0.11546   0.11546 color 1 shaded quad
 3)     H1  -0.32460   0.34680   0.18480 color 4 hollow
 4)     H2   0.21000   0.21000   0.21000 color 4 hollow
```

Graph



Key



Hint: You can have many command windows open and changes in one will update the other windows. If things seem slow, try having fewer windows open.