Guide to making a Crystallography Web Page

This guide requires the use of the following programs and is specific to a Windows OS (some options may differ on other OS).

- Accelrys Materials Studio (v4.3)
- Jmol.jar application
- Dreamweaver (MX 2004)

We will use the simple structure of NaCl (rocksalt) for this example.

Drawing the crystal structure

The Space Group, Lattice Parameters, and the fractional coordinates of at least one of each type of atom in the structure must be known before proceeding.

NaCl

Space Group FM-3M

Lattice Parameters (Å)

A=b=c=5.640

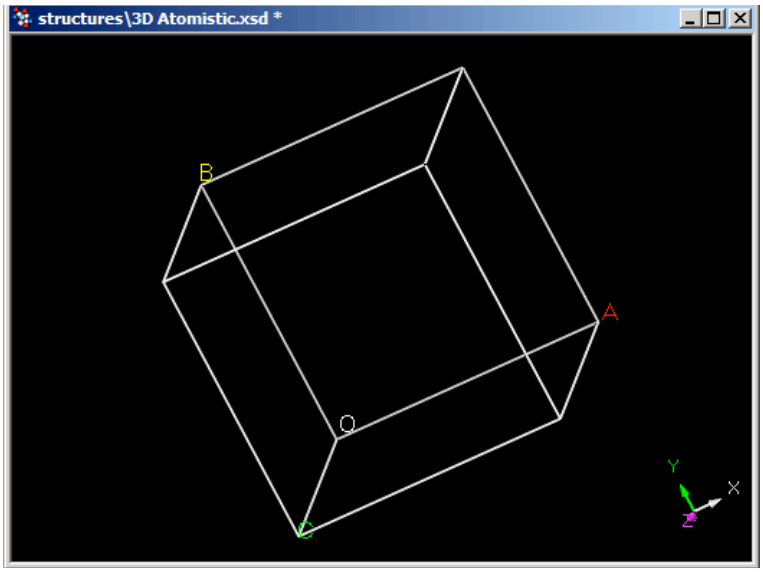
From Materials Studio, select File -> New -> 3D Atomistic.

Build -> Crystals -> Build Crystal...

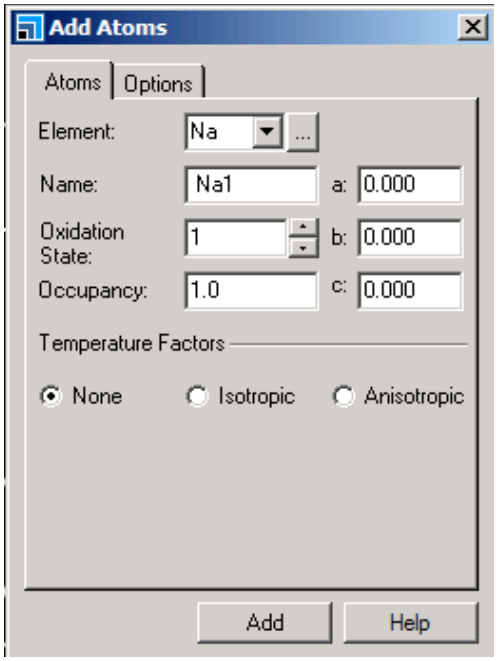
In Space Group tab, Enter group box, enter “FM-3M”.

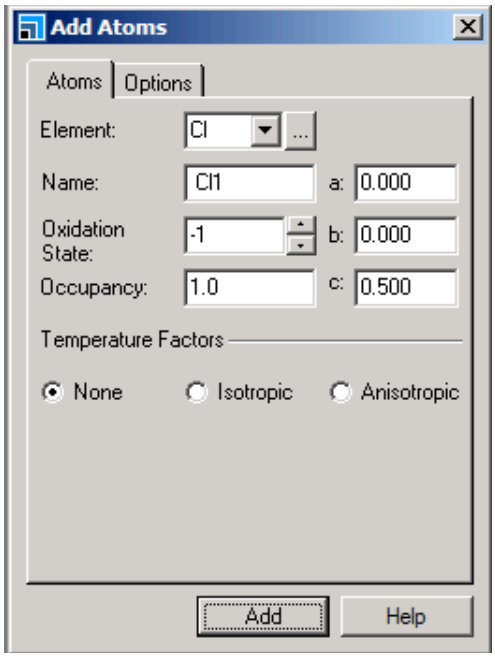
In Lattice Parameters tab, enter the lengths (Å) of a, b and c.

An empty cell should be drawn:

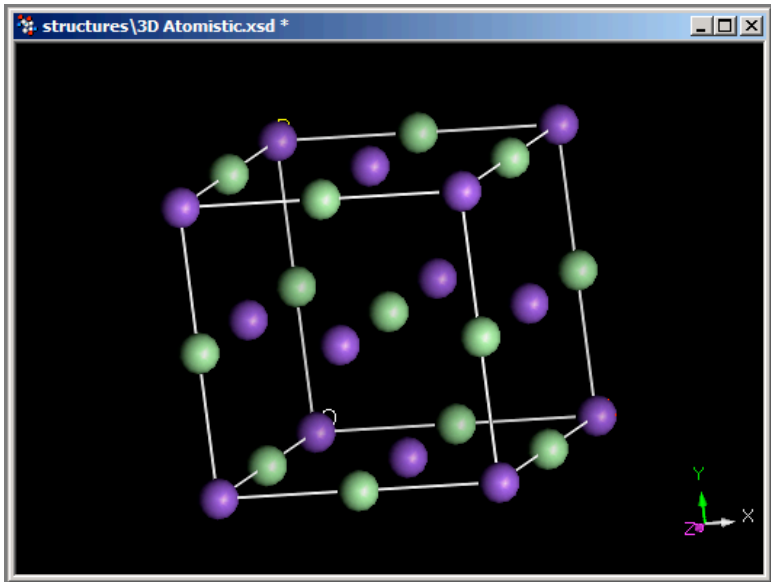


To add atoms, Build -> Add Atoms.



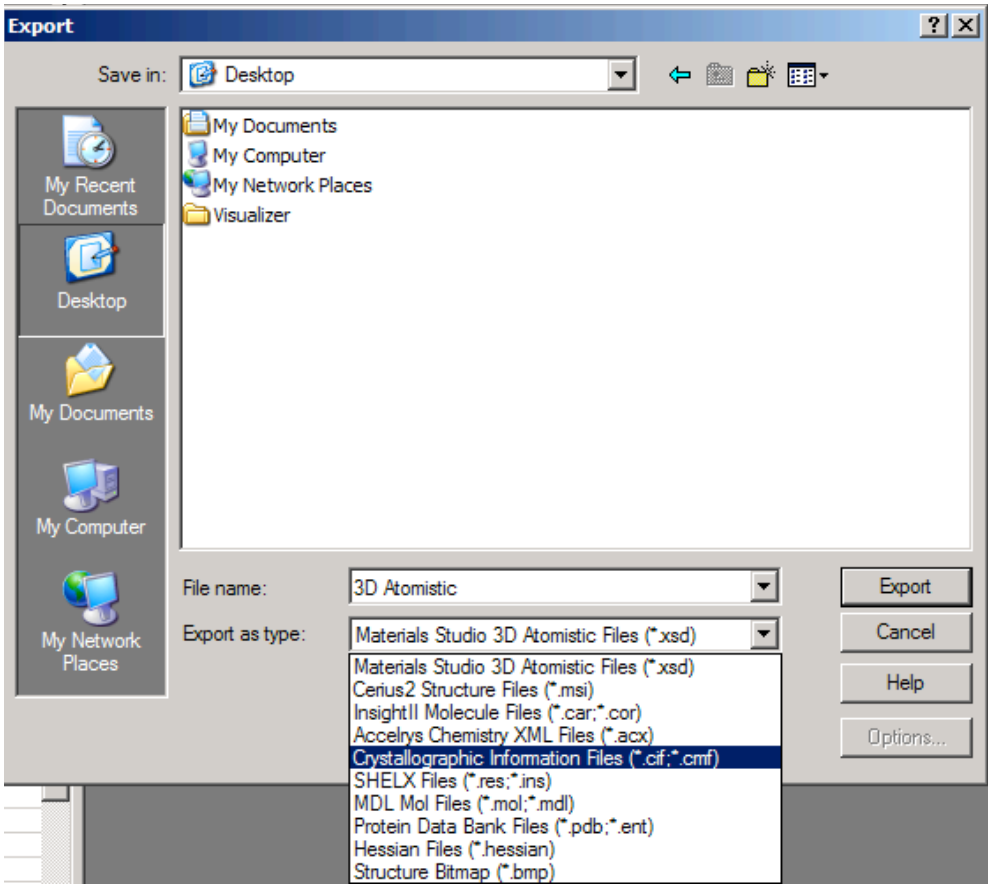


This should give a unit cell of NaCl:



Save the untitled 3D Atomistic document and the export using File -> Export...

Save in desired directory, but ensure that in the “Export as type:” field, Crystallographic Information Files (*.cif, *.cmf) is selected.



Displaying Polyhedra and Unit Cells in Jmol

Testing of Jmol commands can be done in jmol.jar or by using Dreamweaver's "Preview in Browser" option. For simplicity, I will only be showing the most important commands.

(In depth explanation of each Jmol command can be found at Bob Hanson's Jmol interactive scripting documentation: http://chemapps.stolaf.edu/jmol/docs/)

jmolInitialize("./");jmolApplet("500",'load test/table/rocksalt.cif {2 2 2}; boundbox on; moveto 1.0 459 -643 -613 130.38; *connect 2.83 (sodium) (chlorine);* unitcell on; unitcell 0.03; axes 0.03')

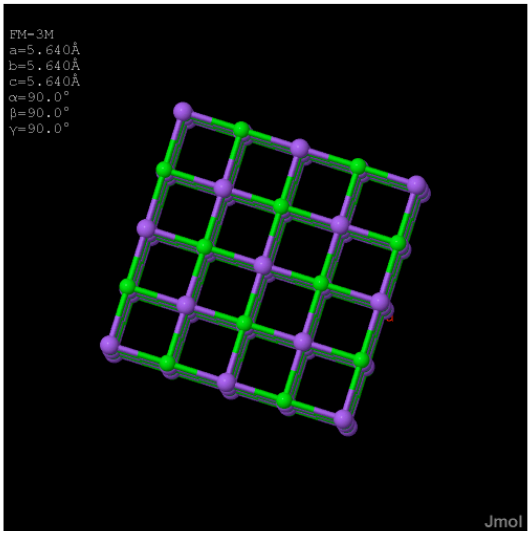
This makes a jmol applet size of 500 and loads the .cif file with 2 x 2 x 2 unit cells.

The moveto command specifies the orientation in which the file is loaded.

Connect X (sodium) (chlorine) draws bonds between all sodium and chlorine atoms within radius X (Å).

This command is not usually needed as Jmol will usually draw the bonds by default.

However, on other occasions, the "command connect (M) (M) DELETE" (where M=metal) may be required to delete unwanted meta-metal bonding.

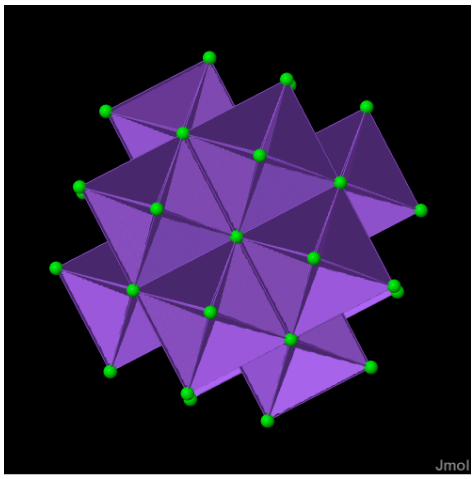


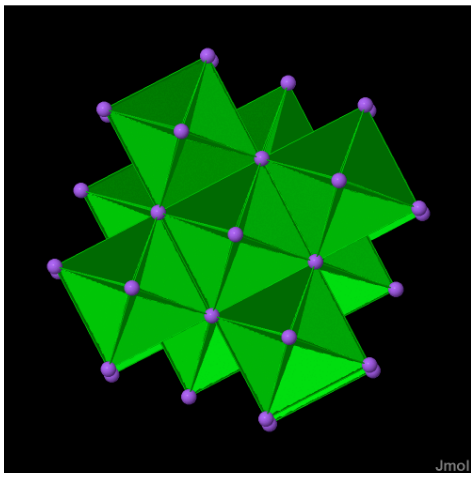
To manipulate the above structure and draw polyhedra, buttons need to be created. (See http://jmol.sourceforge.net/demo/jssample1/)

jmolButton('select *; hide none; centre; boundbox off; unitcell off; axes off; wireframe off; spacefill off; polyhedra off; polyhedra 6 (_Na) to (_Cl) collapsed edges; select (_cl) or connected(6); spacefill 12%; zoom 150; hide atomno=X or atomno=Y or atomno=Z', "Na Polyhedra")

jmolButton('select *; hide none; centre; boundbox off; unitcell off; axes off; wireframe off; spacefill off; polyhedra off; polyhedra 6 (_Cl) to (_Na) collapsed edges; select (_na) or connected(6); spacefill 12%; zoom 150; hide atomno=X or atomno=Y or atomno=Z', "Cl Polyhedra")

(Where X Y Z are atom numbers)





The method of displaying polyhedra from the above is

Polyhedra N (A) to (B)

(Where N is the coordination number of species B around A)

When this fails, other methods include:

select (A); polyhedra N bonds;

Polyhedra are drawn from the bonds around the central atom, A. The number of bonds = coordination around A = N. If bonds are not present, they must be drawn first using the "connect X (A) (B)" command as above.

Polyhedra bonds (A); or **polyhedra bonds (A and not B);**

Related to the command above. This command can be used if there is a fixed number of bonds from central atom A.

select (A); polyhedra radius X;

Polyhedra are displayed, regardless of coordination number, within distance X (Å) from central atom A.

select connected(N); polyhedra bonds (A) distancefactor Y;

If the polyhedra of species A have many faces (i.e. N is large, >8), the distancefactor Y may have to be increased from a default value of 1.85 in order for more faces in a polyhedron to be included.

polyhedra N (displayed);

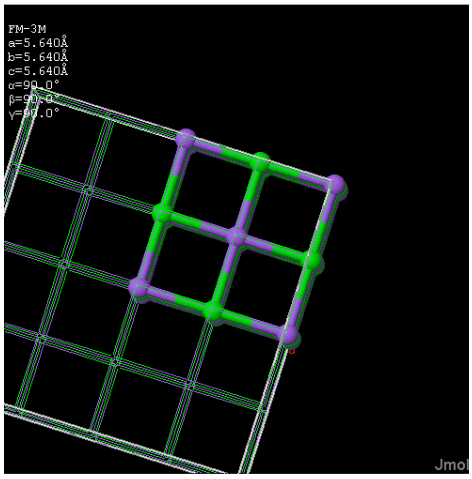
This allows all polyhedra of coordination N to be drawn from the atoms displayed in the Jmol window.

A single polyhedron can also be displayed using the above methods in most cases, but an atom must first be specified as the central atom using "select atomno=X".

select atomno=X or atomno=Y; polyhedra N; etc.

Unit cells can also be highlighted in a structure using similar principles.

select*; hide none; wireframe 0.02; spacefill off; polyhedra off; select unitcell; wireframe 0.2; spacefill 0.4; centre unitcell; zoomto; zoom 200; unitcell on; unitcell 0.03; axes 0.03



The ccp and hcp pages were also created by selecting different sets of atoms, and altering the parameters of wireframe and spacefill commands as above.