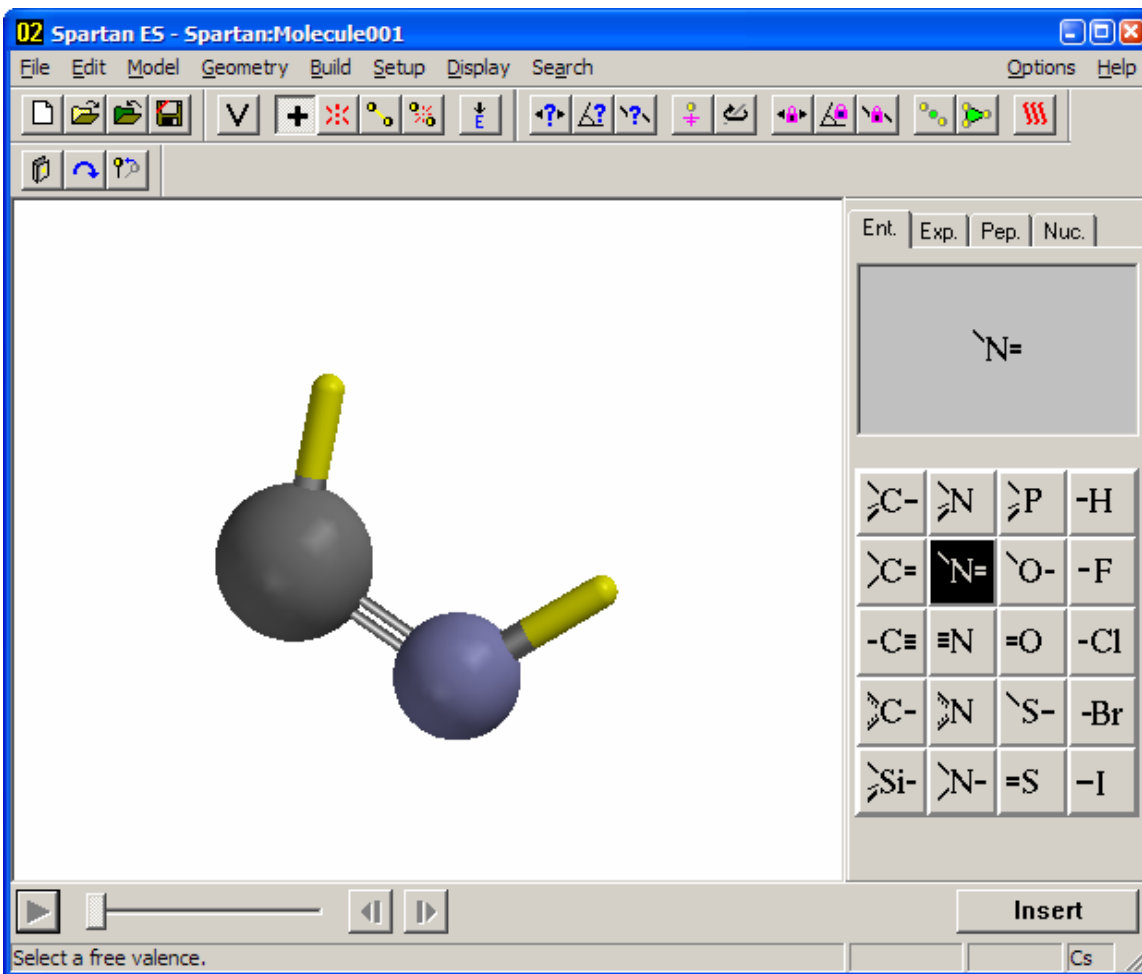


- 1) Click on the **Spartan '02 ES** icon to open the program.
- 2) Under **File**, click on **New**:  
the tools for building molecules appear on the right (see below).



- 3) **Build the molecule**, adding an atom at a time to the appropriate spot.  
Choose the atom with multiple bonds if your molecule includes such bonds.  
Rotate the molecule with the mouse (press and hold the left mouse button),  
or move it (right mouse button) or enlarge it (shift+right mouse button).  
When you have built your molecule, click on the **View** button [V]  
Hydrogen atoms are added automatically to any open (yellow) bond.  
To modify the molecule, atoms may be deleted with the **Delete** [\*] button  
Create bonds between open positions using the adjacent **Make bond** button  
The next button can be used to break a bond.  
The **Add fragment** [+] button reopens the building tool area if it is closed.

4) **Minimize the structure**, using the minimize button [E]

This minimization uses an empirical force field, not a quantum calculation.

The minimized molecule sometimes looks quite wrong: go back and rebuild it.

You can measure bond lengths, valence angles, and torsion angles with the buttons with question marks: press the button, followed by the atoms defining the coordinate.

**Quantum calculations:**

The geometry of the initial minimized (equilibrium) structure may differ a bit from that which would be found using a particular *ab initio* technique. Thus the next step should be minimizing the geometry with a given choice of method and basis set. The new minimized structure is best to look at orbitals or vibrations, or whatever. Since such additional calculations are more cumbersome, they are best not done during minimization.

5) **Find the minimized structure**

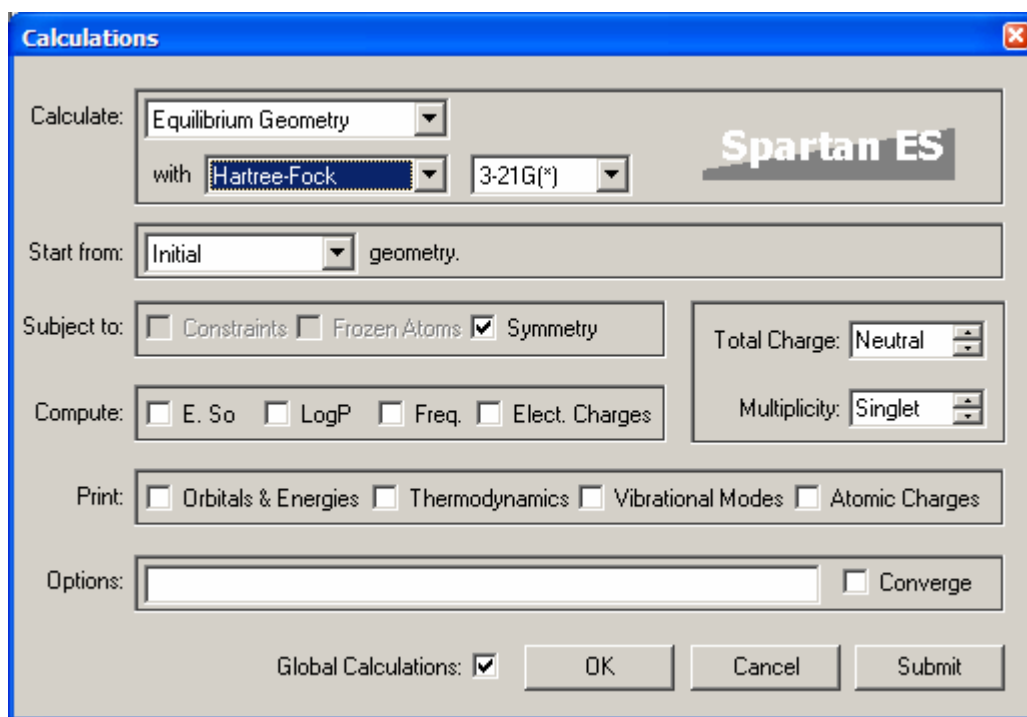
Under **Setup**, press **Calculations**. The **Calculations** window appears (see below)

Choose Calculate: **Equilibrium Geometry**

Choose **Hartree-Fock**, a suitable basis set, and the correct Total Charge and Multiplicity;

Press **ok**. Then under **Setup**, press **Submit**. It will prompt you to save the file:

do so into your folder, using a descriptive name.



When the calculation finishes, the new molecule appears (unless there is some problem).

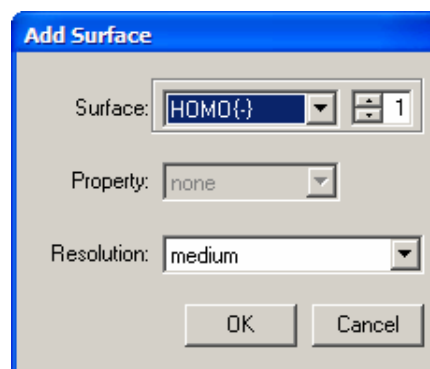
If it stops because there is some problem, look at the output to see what happened:

Display > **Output**.

The output also shows details of the calculation: there will typically be a number of steps (cycles) before the minimum was found. At the minimum, the gradient vector (vector of derivatives of the potential) has zero length. The total energy is given in Hartrees.

If the molecule is large or the initial geometry far off, minimization may take some time.

- 6) **Viewing Orbitals:** Go back to Setup > **Calculation**  
 Choose **Single Point Energy** using the same basis set,  
 and check Print **Orbitals & Energies**.  
 Then before submitting, choose Setup > **Surfaces**.  
 Press **Add**: the **Add Surface** window opens.  
 Select the surfaces you wish to view  
 HOMO = highest occupied MO  
 HOMO-n = n orbitals below HOMO...  
 when you have selected all you wish to view,  
 submit the job: Setup > **Submit**



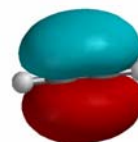
When the job is done, look at each orbital:

Display > **Surfaces**

**Check** the orbital you want to see. You can experiment with Styles:  
**Solid** is good for one orbital (as the HOMO of HCCH at right), but  
 other styles may be useful when looking at combinations of orbitals.  
 Rotate the molecule so you can see the orbital at a good angle.

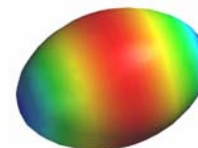
You can copy and paste the image into a Word or other document.

The output shows numerical properties (energies and coefficients) of the orbitals.



Other surfaces can be constructed. Values of one function (such as  
 electrostatic potential) can be displayed on the density surface.

**Example at right:** electrostatic potential on acetylene.



- 7) **Vibrations:** Go back to Setup > **Calculation**  
 Choose **Single Point Energy** using the same basis set,  
 and check Compute: **Freq.** and Print **Vibrational Modes**.  
 Submit.  
 When the job is complete, Display > **Vibrations**.  
 The **Vibrations** window opens.  
 Listed are frequencies and symmetries of each normal mode.  
 If a frequency starts with *i*, it is imaginary  
 this means that your geometry is not a minimum.  
 (sometimes, as at right, symmetries are not found).  
 Click on a mode to see it animated.  
 You can view the numerical results in the output.

Frequency	Type
902.73	???
902.77	???
918.73	???
918.76	???
2234.07	SG+
3595.19	SU+
3718.49	SG+

Amp: 0.500 Å Steps: 11

Make List

**There are many other things you can do:** freeze part of a molecule, find transition states, etc.  
 Under **Options**, you can play around with colors as well as monitor ongoing calculations.  
 Experiment! Consult the manuals in 613 Altschul.

**A strong recommendation:**

If you are doing several kinds of calculations on a molecule, close Spartan after each one, and start giving a different file name. This way all the results will be saved.