In addition to the basic operations of the CAChe software described in the document Molecular Modeling, you need to know how to (a) set or determine the formal charge of an atom and (b) set or determine the hybridization of an atom.

**FORMAL CHARGE**

Atoms in molecules and ions often bear an electric charge. The oxidation number of an atom is one way to characterize atom charge, and another, more useful way when discussing covalently bonded molecules or ions, is formal charge. The formal charge of an atom in a molecule or ion is calculated from the formula

\[
FC = \text{Group number of atom} - \left(\text{number of lone pair electrons surrounding the atom}\right) + \frac{1}{2}(\text{number of bonding electrons})
\]

This formula assumes that the atom begins as a cation whose charge is equal to the element’s group number in the periodic table minus the valence electrons. Thus, a C atom begins as C\(^{4+}\) and O begins as O\(^{6+}\). When placed in the molecule or ion, however, the atom “recaptures” electrons. We assume that it recaptures electrons localized on the atom as lone pair electrons. Further, we assume that one-half of the electrons in bonds formed by the atom are recaptured. Thus, in the hydroxide ion, the O atom has 6 lone pair electrons and 1 electron recaptured from the O–H bond. The O atom formal charge is -1. This is also the charge on the OH\(^-\) ion because the formal charge of H is 0.

When building a molecule using the CAChe software, one must set the formal charge of the atoms in the molecule so that the electronic structure is built properly. Therefore, the first step is to draw the electron dot structure of the molecule or ion and calculate the formal charges. Taking the nitrate ion as an example, you see the formal charge on the central N atom is +1, whereas that of each singly bonded O atom is -1.
ATOM HYBRIDIZATION

The bonds in the nitrate ion are at the corners of a planar triangle, whereas the valence electrons of the N atom are located in a spherical s orbital and dumbbell shaped p orbitals, which lie 90° relative to one another. Linus Pauling proposed that the N orbitals actually used in forming the sigma (σ) bonds in the planar triangle are composed of a new set of orbitals that are formed by hybridizing the s and two of the three p orbitals into a new set of hybrid orbitals. Each orbital in this new set is labeled \( sp^2 \) to indicate that it is composed of a portion of an s orbital and portions of two p orbitals.

Directions for the Macintosh Platform

Step 1: In the CAChe system, draw a structure having N in the center with two singly-bonded O atoms and one double-bonded O atom.

Step 2: Go to the TOOL menu and select the ATOM tool. Hold down the OPTION key and click on the N atom. This will bring up as periodic table with N highlighted. Type the formal charge into the box marked “Charge” and click OK. When you return to the screen with the nitrate ion you will see the N atom is now marked with a +1 charge.

Now use the same method to set both singly-bonded O atoms to a -1 charge.

Step 3: Save the nitrate ion with the proper formal charges.

Step 4: Go to the TOOL menu and choose the SELECT Tool. Make sure all the atoms are “active” (that is, none are “greyed out.”). Use the COMPREHENSIVE command in the BEAUTIFY menu to build the ion in its correct geometry.

Step 5: With the molecule model still on the screen, go to the VIEW menu and select ATOM SHAPE. The following dialog box will open.

When you save molecules, please save them in a new folder with your name on it. When you are finished with the computer at the end of the day, please delete your folder by dragging to the trash.
When the boxes “Element and charge” and “Configuration” have been checked, the nitrate ion will now appear with atom formal charges and orbital hybridizations marked on each atom.

**Directions for the Windows Platform**

**Step 1:** Open a new Workspace in the CAChe system. To construct a model of the nitrate ion, draw a structure having N in the center with two singly-bonded O atoms and one double-bonded O atom.

**Step 2:** Click on the N atom and then click in the third box from the left to raise the formal charge to +1. Similarly, click on the singly bonded O atoms and lower their charge to -1.

**Step 3:** Beautify the model and save it, preferably in a folder having your name.
Step 4: To ensure that the formal charges and atom hybridizations appear on the model on the screen, go to the VIEW menu. When you open ATOM ATTRIBUTES, a many-layered dialog box appears. Click on the tab marked LABEL. As seen in the figure below, you can check “Atomic symbol,” “Hybridization,” and “Charge” to automatically label atoms in models. If you click “Make default” and then “OK” before closing this box, the symbols, hybridization, and charges will always appear.

The nitrate ion model will not appear on the screen as seen here.