Molecular Representations and Tables of Common Polyatomic Ions

Graphical computer modeling has greatly improved our ability to represent three-dimensional structures. One of the goals of graphical computer modeling is to create a computer-generated model that appears to be three-dimensional. By replicating the effect of light on three-dimensional objects, computers can give the impression of depth to simulate a three-dimensional appearance. The use of interactive molecular viewing (*e.g.*, using the Chime program) has enhanced our understanding of molecular structure, especially in the biochemical area. By interactively rotating the molecules, a clear picture of the three-dimensional structure emerges. In addition, this increases our chemical intuition because it teaches us to look at two-dimensional images and visualize their three-dimensional structure in our brains.

This course uses different types of structural representations, such as **2D-ChemDraw, stick, CPK, and ribbon,** to illustrate the structure of molecules and macromolecules. PDB files are also available for viewing the molecules interactively. Figure 1 is a segment of an alpha helix polypeptide string shown in four different types of computer-generated molecular representations. Although all four representations depict the same molecule, each has a distinct appearance and offers different information about the molecule's structure.

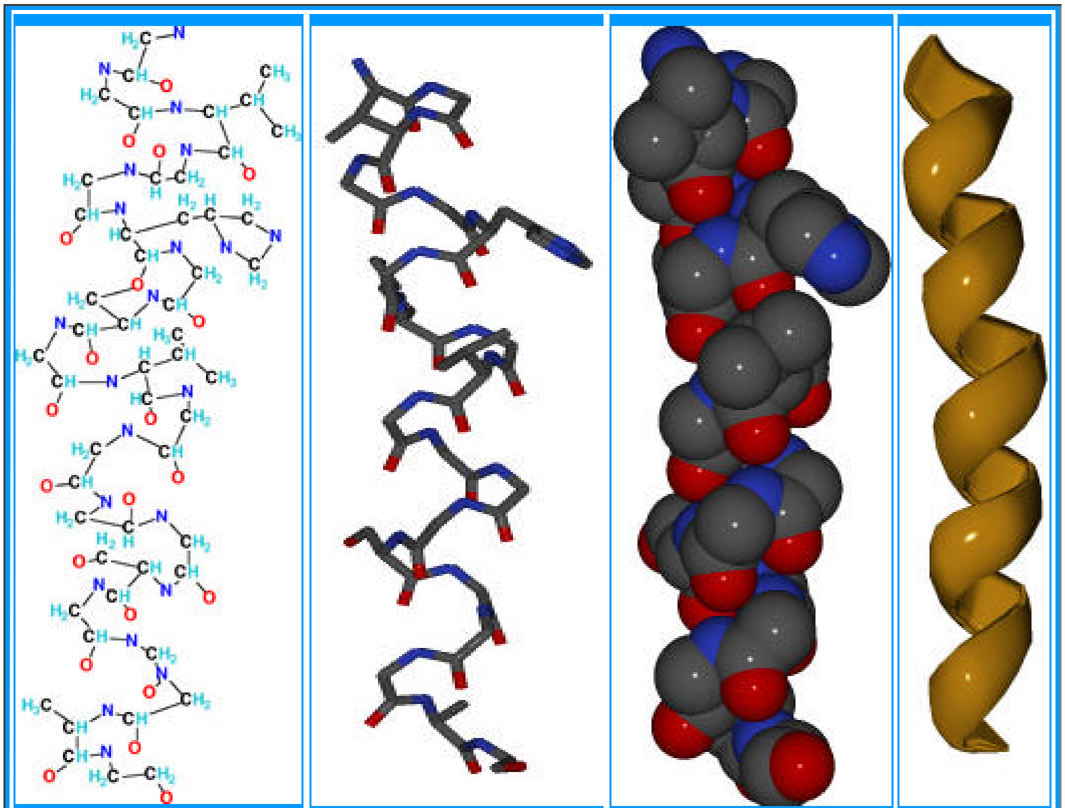


Figure 1 A segment of an alpha helix

The representations from left to right are 2D-ChemDraw, stick, CPK, and ribbon models. In the 2D-ChemDraw, stick, and CPK representations, carbon atoms are shown in gray (black), nitrogen atoms are shown in blue, and oxygen atoms are shown in red. In this figure, hydrogen atoms (light blue) are shown in the 2D-ChemDraw representation but hydrogen atoms are not shown in the other representations.

By examining the four representations in Figure 1, you can see that each picture tells us something different about the structure of the molecule. For instance, if we wanted to know how the atoms in an alpha helix are connected to one another, we would use 2D-ChemDraw or stick representation. To see the relative sizes of the atoms in an alpha helix, we would use the CPK (or space-filled) representation. Descriptions of the four types of representations, their major strengths, and their drawbacks are given in the table below.

Type of Representation	Description of Representation	Information Depicted Particularly Well by Representation	Drawbacks of Representation
2D-ChemDraw	Shows labeled atoms and bonds connecting atoms in a flat representation.	Shows connectivities between atoms in small molecules; can also include lone pairs (i.e., Lewis-dot structures).	Difficult to interpret for larger molecules; does not give a good idea of the molecule's three-dimensional structure.
STICK	Shows the bonds between atoms as three-dimensional "sticks" that are often color-coded to show atom type.	Shows connectivities between atoms; gives some idea of the molecule's three-dimensional shape.	Does not depict the size (volume) of the molecule or its constituent atoms, and hence gives a limited view of the molecule's three-dimensional shape.
CPK[1]	Shows atoms as three-dimensional spheres whose radii are scaled to the atoms' van der Waals radii.	Shows the relative volumes of the molecule's components; usually a good indicator of the molecule's three-dimensional shape and size.	Difficult to view all atoms in the molecule and to determine how atoms are connected to one another.
RIBBON	Shows molecules with a "backbone" (e.g., polymers, proteins) and depicts alpha helices as curled ribbons.	Shows the secondary structure (such as locations of any alpha helices) of a protein.	Used for proteins and other polymers; does not show individual atoms and other important structural features.

Tables of Common Polyatomic Ions

The tables below list common polyatomic ions that you will be using throughout this General-Chemistry laboratory series (Chem 151-152). These ions are separated by charge on the ion into four (4) different tables and listed alphabetically within each table. For each polyatomic ion, the name, chemical formula, two-dimensional drawing, and three-dimensional representation are given.

The three-dimensional structures are drawn as CPK models. CPK structures represent the atoms as spheres, where the radius of the sphere is equal to the van der Waals radius of the atom; these structures give an approximate volume of the polyatomic ion. In these tables, the three-dimensional structures have all been drawn to the same scale; therefore you can compare their relative sizes. In addition, the atoms in the CPK structures have been color-coded to match the two-dimensional drawings for easier comparison. To view the ions interactively, please use Chime. For

[1] It is also called space-filling models. CPK stands for the names of the three scientists who designed and developed this model to represent biological macromolecules in 1960.

viewing and rotating the ions listed in the tables below, please click on the appropriate three-dimensional structure.

Table 1: Cations (+1 Charge)

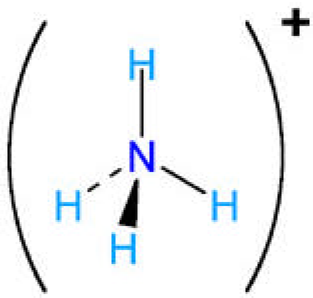
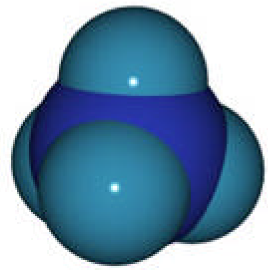
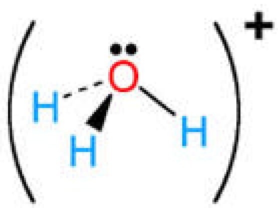
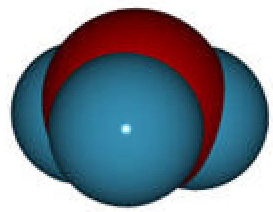
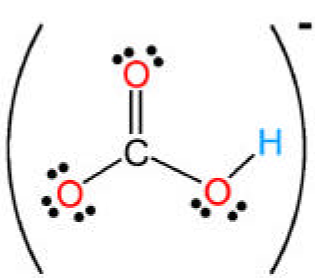
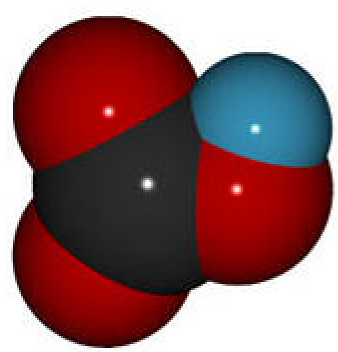
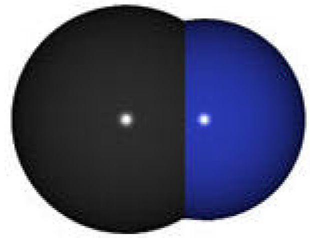
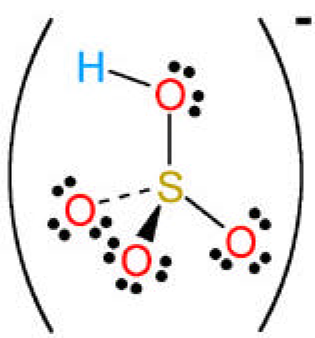
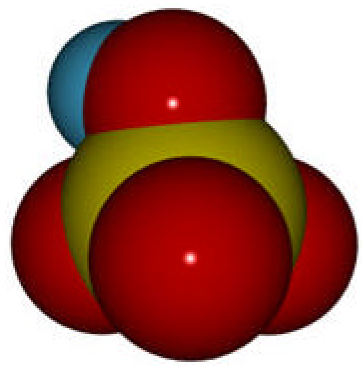
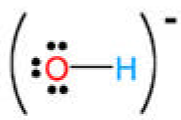
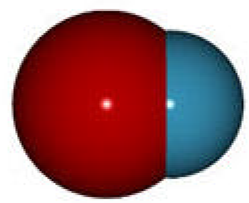
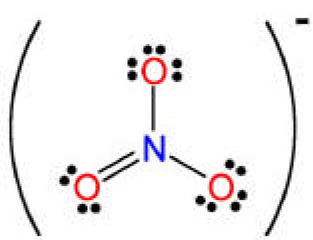
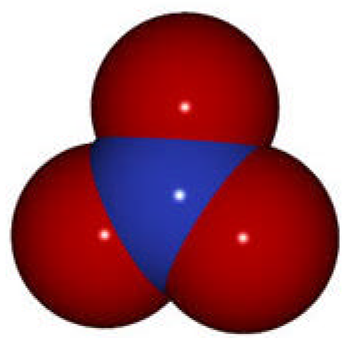
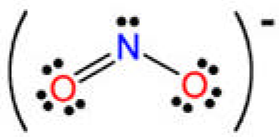
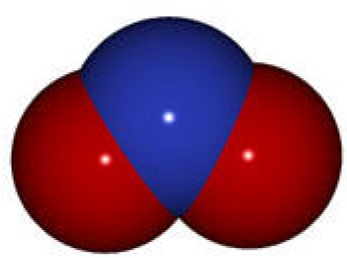
Ion	Two-Dimensional Structure	Three-Dimensional Representation
Ammonium NH_4^+		
Hydronium H_3O^+		

Table 2: Anions (-1 Charge)

Ion	Two-Dimensional Structure	Three-Dimensional Representation
Bicarbonate HCO_3^-		

Cyanide CN^-		
Hydrogen Sulfate HSO_4^-		
Hydroxide OH^-		
Nitrate NO_3^-		
Nitrite NO_2^-		

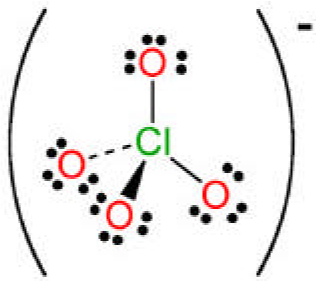
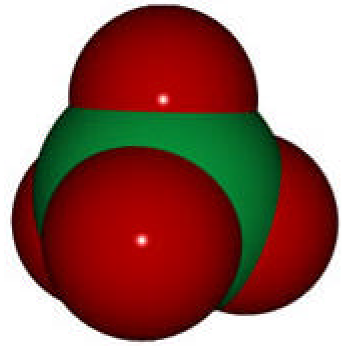
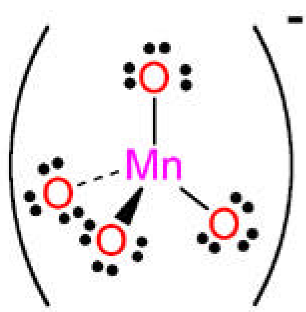
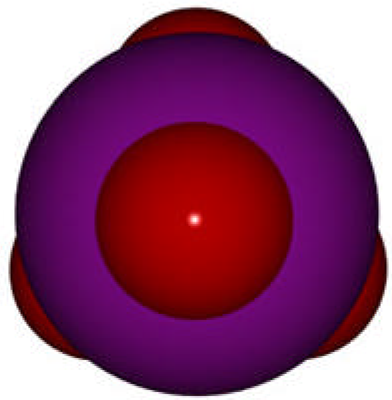
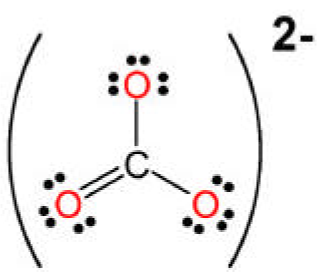
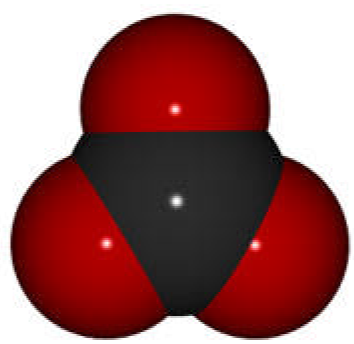
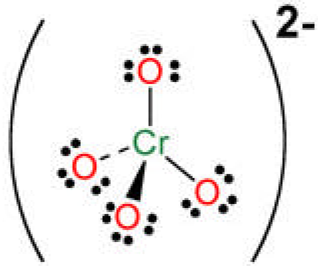
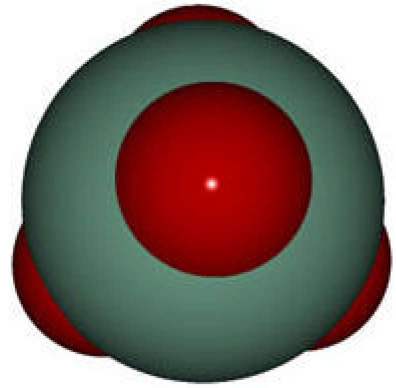
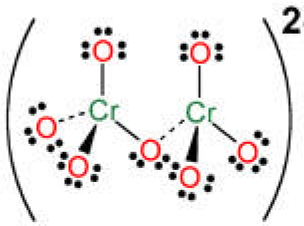
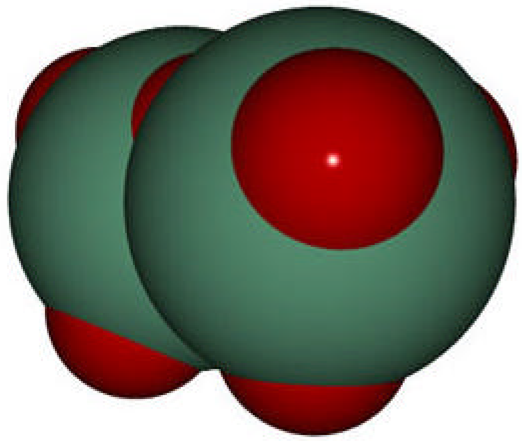
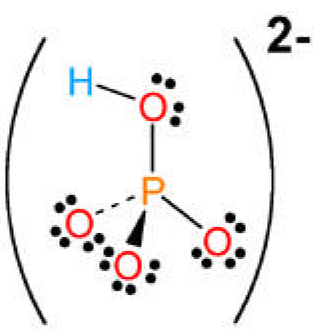
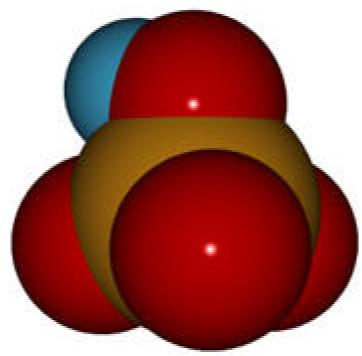
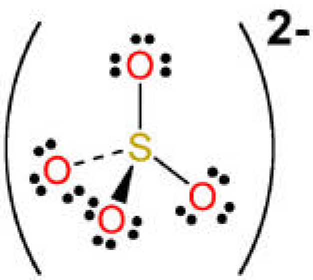
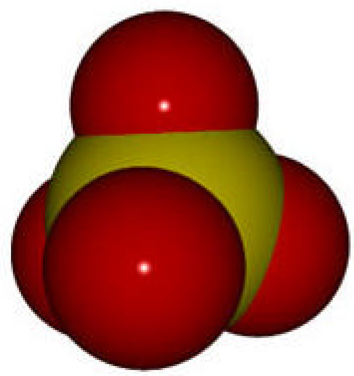
Perchlorate ClO_4^-		
Permanganate MnO_4^-		

Table 3: Anions (-2 Charge)

Ion	Two-Dimensional Structure	Three-Dimensional Representation
Carbonate CO_3^{2-}		

<table>
<tr><th></th><th></th><th></th></tr>
<tr><td>Chromate
CrO_4^{2-}</td><td>
</td><td></td></tr>
<tr><td>Dichromate
$Cr_2O_7^{2-}$</td><td>
</td><td></td></tr>
<tr><td>Hydrogen
Phosphate
HPO_4^{2-}</td><td>
</td><td></td></tr>
<tr><td>Sulfate
SO_4^{2-}</td><td>
</td><td></td></tr>
</table>

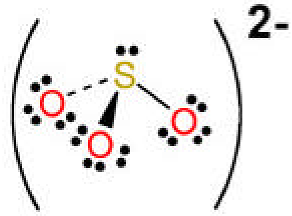
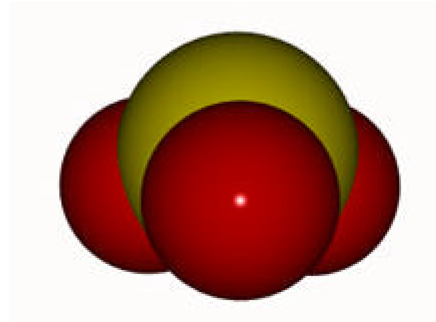
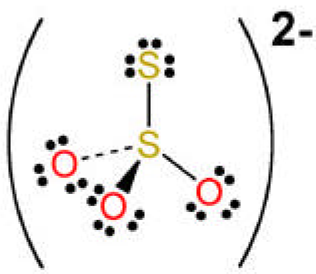
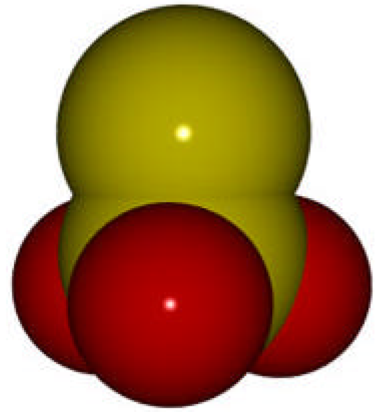
Sulfite SO_3^{2-}		
Thiosulfate $S_2O_3^{2-}$		

Table 4: Anions (-3 Charge)

Ion	Two-Dimensional Structure	Three-Dimensional Representation
Phosphate PO_4^{3-}