Representative Example of Modeling Using Ball and Stick Molecular Models

In assembling molecular models of the kind we are considering, it is usually desirable to use a systematic approach. The method suggested below parallels the method for writing Lewis structures that we have discussed in class. We will illustrate this method by developing a model for formaldehyde, CH_2O.

1. *Determine the total number of valence electrons and select the appropriate number of*

pegs. Recall that for the "main group elements," (of the Periodic Table) which we will be using (H, C, N, O, F, S, Cl, Sb, Xe, and I), the number of valence electrons on an atom is equal to the group number. If the structure to be constructed has one or more **electric charges** (+ or -), **add one electron to the total for each negative charge and subtract one electron for each positive charge.** Each peg in our models represents two electrons, so once you have determined the total number of electrons, count the number of pegs to be used in your structure.

For formaldehyde each **H** contributes one valence electron, the **C** contributes four valence electrons and the **O** contributes six valence electrons to the overall structure. This yields a total of 2(1) + 4 + 6 or 12 valence electrons. Therefore, our structure will require six pegs.

2. *Select the appropriate wooden balls and deduce a skeletal structure for the molecule*.

Each hydrogen atom in our models is represented by a yellow ball with one hole (accommodating one electron pair) and, initially, each "heavy atom" will be represented by a black ball having four holes (accommodating four electron pairs, an "octet"). Thus select one ball of the appropriate type for each atom in your molecular formula.

The skeletal structure is the **sequence of attachments (or the connection of atoms to one another) within the molecule**. Frequently this can be discerned from the order in which the atoms are written in the molecular formula. Often the first atom in the formula is the central atom (especially if it is the least electronegative element) with those following all being attached to it. For more complex structures (e.g., ethyl alcohol considered below) the skeletal structure will sometimes be suggested by subdivisions in the molecular formula (CH_3CH_2OH for ethyl alcohol). Sometimes there will be several possible and/or reasonable skeletal structures for a given molecular formula. Such molecular formulas are said to have several possible structural isomers (discussed below). If your skeletal structure requires more than four atoms to be attached to a central atom, that central atom will require an "expanded octet". In such cases, replace the black ball (4 holes) with an appropriate expanded octet ball (5 holes, light blue) and proceed to Step 3.

For formaldehyde we will require two yellow balls (two H atoms) and two black balls (one C and one O atom). We can choose a skeletal structure having **C** (black ball with four holes) as the central atom with the **H** atoms (yellow balls with one hole) and the **O** atom (black ball with four holes) attached to it.

3. *Assemble a single-bonded structure for the molecule.*
Simply connect the adjacent atoms in your skeletal structure by inserting each end of a wooden peg into holes in adjacent atoms. If there are **no empty holes** in any of the atoms **and no unused pegs** after doing this, the **structure is complete**,1 proceed to Part B. If there are empty holes or extra pegs, proceed to step 4.

For formaldehyde, three pegs are required and our single-bonded structure will have three of the holes in the **C** filled with pegs attached to the **O** and two **H** atoms. In this case there is one empty hole in the **C**, there are three empty holes in the **O** and there are three unused pegs. Thus, we proceed to Step 4.

4. *Add lone pairs.* If you have additional pegs, place them in the empty holes. If **all of the holes are filled and all of the pegs are used** at this point, the **structure is complete**;[2] proceed to Part B. If there are empty holes or extra pegs, proceed to step 5.

For formaldehyde, we can fill three of the four empty holes. Thus, we are left with one empty hole on either the **C** or the **O** atom so we proceed to Step 5.

5. *Add multiple bonds and/or expand octets.*
(a) ***If there are empty holes***, your molecule is called **unsaturated** since there are insufficient electrons to fill the octets of all atoms. To reach octets, some atoms will need to share more than one electron pair with one or more of their neighbors. A double bond can be created by using a lone pair of electrons on one atom to help fill an empty hole on an adjacent atom (using two lone pairs from a single atom to fill two empty holes on a single adjacent atom produces a triple bond). To locate the most appropriate sites for multiple bonds, **arrange the lone pairs in your single bonded structure so that each atom with an empty hole is adjacent to at least one atom with at least one lone pair**. To complete the multiple bonds, we require more flexibility than the wooden pegs can provide, so we will use springs to form the double and triple bonds. **At each site where there is an empty hole and an adjacent lone pair, replace both the lone pair peg and the peg representing the bond between the adjacent atoms with springs**. This will provide the structural flexibility to allow you to **create the multiple bond by inserting the free end of the lone pair spring into the empty hole on the adjacent atom**. Complete octets of all atoms (fill all empty holes) by creating multiple bonds. Usually there will be more than one arrangement of multiple bonds that will fill all of the holes. At this point in our exercise, any one of the possible multiply bonded structures is sufficient. **Your structure should now be complete**; go to Part B.

For formaldehyde we can use a structure with an empty hole on **C** and three lone pairs on **O** or one with an empty hole on **O** and one lone pair on **C**. In either case we replace the **c—O** bond peg and one lone pair with springs and then **form a double bond**

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[2]Such completely single bonded molecules are said to be **saturated molecules** since they have all of the electrons they can accommodate without expanding the octet of one of their atoms.

between C and O by connecting them with the two springs. This completes the structure for formaldehyde since all holes are filled and all pegs and springs are used.

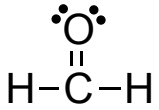
(b) ***If you have additional pegs.*** Your molecule has more electrons than can be accommodated by octets on all heavy atoms so that the octet of one or more of the atoms in the structure will need to be "expanded". Atoms from the third row of the Periodic Table or below can accommodate more than eight valence electrons; thus they can have "expanded octets." Select the atoms in your structure which can have expanded octets, and replace them in the structure with a light blue (5 holes — 10 electrons) ball. Fill the extra holes with your unused pegs.

Interpretation of Properties Using Ball and Stick Molecular Models

1. *Draw the Lewis Dot Formula for your Model.*

Simply write down the atoms, bonds, and lone pairs from your model built in Part A. This exercise should help you gain a sense of the three-dimensional structure represented by Lewis dot formulas. Ultimately, it will be very useful for you to use the two dimensional Lewis formulas to visualize three-dimensional structures without the aid of "ball and stick" models. Lewis structures are much quicker and easier to produce and when you can "see them in three dimensions" they will be very powerful reasoning tools for you to use in predicting the shape and properties of molecules.

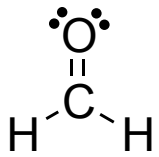
For formaldehyde the Lewis dot formula is:



2. *Examine the Molecule's Molecular Geometry and describe the general overall shape of the molecule.*

Do the outer most atoms form a recognizable solid form (e.g. a cube, a pyramid, a tetrahedron, a bipyramid, an octahedron, etc.)? Is the molecule flat (planar) or are the atoms all in a line (linear)? If the molecule is planar, does it have an easily recognizable regular shape (e.g., a triangle, a square, a pentagon, etc.)?

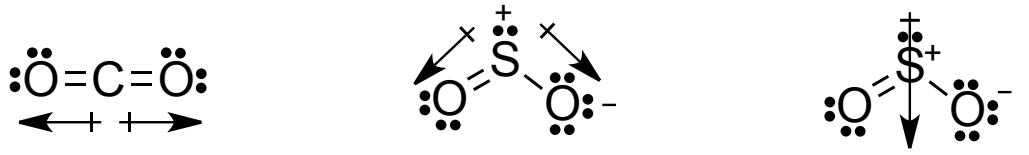
Formaldehyde is flat (all of its atoms lie in one plane) with its peripheral atoms forming the vertices of a triangle. Such a structure is called trigonal planar:



3. *Predict the Molecule's Polarity.*

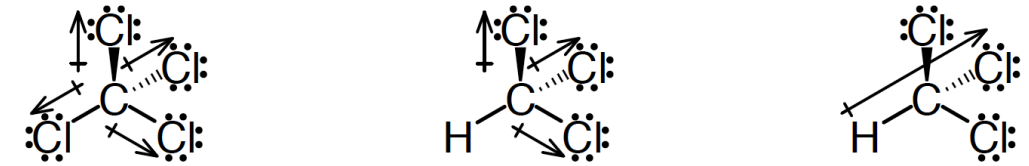
Polar bonds are formed between two atoms with different electronegativities. The more electronegative atom pulls more than its fair share of electrons towards it to give it a partial negative charge. The less electronegative atom will have some electron density pulled away from it, so it will be partially positively charged. This polar bond creates a dipole (two poles) for that part of the molecule. The total dipole moment of the molecule is the vector sum of all the bond dipoles. For example, both CO_2 and SO_2 have polar bonds. However, the bond dipoles in carbon dioxide oppose each other and cancel out since CO_2 is a linear molecule (the dipoles can be considered to be vectors, in this case,

of exactly the same magnitude in opposite directions). In SO_2 the bond dipoles do not cancel, therefore, the whole molecule is polar. In the pictures, we sometimes use arrows to show the dipole, with the arrowhead pointing in the direction of the partial negative charge and the partial positive charge depicted with a "plus" on the other end of the arrow as shown below.



Bond dipoles cancel | Bond dipoles do not cancel | Net molecular dipole

Symmetrically substituted linear, trigonal planar, tetrahedral, trigonal bipyramidal, and octahedral molecules are non-polar. As another example, CCl_4 is non-polar while $CHCl_3$ is polar.



Bond dipoles cancel | Bond dipoles don't cancel | Molecular dipole

nonpolar | ***polar***

A small electronegativity difference, such as that between **C** (2.5) and **H** (2.1) is not sufficient to create a noticeable bond dipole. However, the electronegativity difference between **C** (2.5) and **O** (3.5) is large and the **C-O** bond is markedly polar.

Does your molecule contain polar bonds? If so, which end of each polar bond is more positive and which is more negative? From the shape noted in step B.2 above, predict whether the molecule as a whole is polar. If you believe it to be polar, indicate the direction of the molecule's dipole moment on the Lewis structure you drew in B. 1, above.

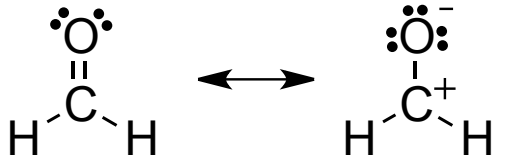
In formaldehyde the **C-O** bond is polar, with the **C** atom partially positively charged and the **O** partially negatively charged. The **C-H** bonds are essentially nonpolar. Thus, formaldehyde is a polar molecule with a net dipole mirroring the **C-O** bond polarity.

4. Examine the Molecule's Potential for Resonance.

If your molecule has multiple (e.g. double and triple) bonds, then resonance is possible. If it is **possible to arrange the multiple bonds in more than one way while maintaining the same skeletal structure**, then each of the possible Lewis structures is a resonance structure. In such cases, the actual structure of the molecule is best represented by an average of all of the resonance structures weighted such that the more reasonable resonance structures contribute more to the average structure than do the less reasonable ones.

There is only one place for the double bond in formaldehyde. One could break up the double bond in formaldehyde to produce a less stable structure containing fewer bonds

and separated charges (see below). Such a structure, although possible, will contribute less to the resonance hybrid than the structure containing a double bond. To calculate the formal charge (FC) on an atom, use the formula: **FC = valence electrons – ½ bonding electrons – nonbonding electrons.**



More stable form Less stable form

5. *Examine the Molecule's Potential for Structural Isomerism*.

If it is possible to arrange the atoms of your molecule in another skeletal structure that is different from the one chosen in Part A.2, then its molecular formula does not describe a unique molecule. Two or more structures that have the **same molecular formula** but **different skeletal structures** (sequences of attachment of atoms) are called **structural isomers**. Note, if there is only one possible structure, there are no isomers. If your molecule has structural isomers, build a model of at least one of them and compare it to your original model.

Is it possible to arrange the atoms of formaldehye, CH_2O, in another way making sure that no formal charges are accumulated any atom and the octet/duet rule is followed? Think and decide.