Molecular Shapes

To be used with https://chemapps.colostate.edu/dli/molecular-shapes/molecular-shapes.html and https://chemapps.colostate.edu/dli/molecular-shapes/molecular-shapes-expanded.html

These two web sites are build with the molecular visualization tool JSmol. JSmol is build from Jmol (Jmol: an open-source Java viewer for chemical structures in 3D, http://www.jmol.org/). JSmol uses Javascript, a scripting language used to build interactivity in the modern web.

This exercise is meant to be open ended where you can explore the set of molecules provided in order to learn about molecular shape. There are three panels allowing you to compare the same molecule with different representations or three different molecules emphasizing different aspects of shape and structure. You can rotate the molecules around to get a good sense of their three dimensional shape by simply click-dragging (clicking on the molecule and moving the mouse (or moving around on a trackpad). Other actions are translation (shift-double-click-drag) zooming in or out (shift-click-drag or just zoom drag (after selecting a frame)), and rotating around the z-axis (of the screen) (option-click-drag). You should routine perform these actions, especially rotating (click-drag) every time you see a molecule to visualize its three dimensionality. You can all so show them with different representations. 0% spacefill is a stick representation, 20% is a ball-and-stick representation, and 80% is the spacefilling model representing the space occupied by the electron cloud. Turn off and on the spin function to help with a three dimensional visualization. Turn off and on the bond angles to see the differences between the various classes of molecules. Lone pairs are shown as small pink atoms—turn them on and off to see the difference between the electron arrangement and the molecule shape based on atoms alone.

Part 1

Here are some comparisons you should try for the first link given *(*molecular-shapes.html*)*. You should draw the Lewis structure for each 3D structure that you see. None of these molecules have expanded octets.

Choose methane, ammonia, and water (the default view), respectively, for the three panels. Counting lone pairs (methane with none, ammonia with one, and water with two) these structures are all based on the tetrahedral structure with roughly 109.5˚ bond angles. Notice how the bond angles change as lone pairs are added.

Choose beryllium difluoride, boron trihydride, and methane, respective, for the three panels. These molecules represent the linear, trigonal planar, and tetrahedral shapes. Note especially, the two-dimensionality (the planarity) of boron trihydride, and the linearity of beryllium difluoride. The first two of these are exceptions to the octet rule

Choose carbon dioxide, formaldehyde, and methane, respectively. These molecules also represent the linear, trigonal planar, and tetrahedral shapes, but with more common molecules some of which have double bonds. Note especially, the two-dimensionality (the planarity) of

formaldehyde, and the linearity of carbon dioxide.

Choose methane, ethane, and propane, respectively. In more complicated molecules (e.g. ethane and propane), chemists describe the shape around each central atom, i.e. each of the two carbons in ethane and each of the three carbons in propane. In each case the carbon with four single bonds and no lone pairs is tetrahedral

Choose ethane, ethylene (ethene), and acetylene (ethyne), respectively. Note especially the planarity of ethylene and the linearity of acetylene.

Choose ethanol and water, respectively. Note how the alcohol group has a similar shape to water.

Part 2

Here are some comparisons you should try for the second link given (molecular-shapes-expanded.html). These molecules have expanded octets and represent the shapes based on trigonal bipyramidal and octahedral structures. Again, you should draw the Lewis structure for each 3D structure that you see.

Choose methane, phosphorus pentachloride, and sulfur hexafluoride (the default view), respectively. These represent the tetrahedral, trigonal bipyramidal, and octahedral structures. Orient them so you see why they are named what they are, i.e. look for the 3D geometrical shape by envisioning lines connecting the outer atoms (not the central atom). Check out the bond angles. Distinguish between axial and equatorial atoms in the trigonal bipyramidal structure.

Choose chlorine trifluoride, sulfur tetrafluoride, and triioide ion, respectively, for the three panels. These represent the T-shaped, seesaw, and linear structures found in the trigonal bipyramidal electron arrangement group. Note that the lone pairs are always found in the equatorial position. Note how the bond angles deviate from expected values based on the lone pairs.

Choose sulfur hexafluoride, bromine pentafluoride, and xenon tetrafluoride, respectively, for the three panels. These represent the square pyramidal and square planar structures found in the octahedral electron arrangement group. Again, note the position of the lone pairs and the bond angles.