# MODELLING MOLECULAR SHAPES

## Introduction

As atoms and molecules are so small, it can often be helpful to use computer simulations in order to help visualise them and understand them at a deeper level. In this experiment you will use two separate modelling programs to model the three dimensional shapes of a variety of molecules. One is a simple simulation produced by the University of Colorado's PhET team who produce a range of excellent simulations of scientific phenomena. The second program is the freeware version of a program by ACDLabs called ChemSketch which in addition to being able to make professional quality chemical equations and diagrams to put in your lab reports, also includes a 3D-modelling program.

## Part 1: The PhET Simulation (record observations etc in the provided table)

1. Go to http://phet.colorado.edu/en/simulation/molecule-shapes and either run or download and run the Molecule Shapes simulation.
2. On the 'Model' tab have a play to familiarise yourself with the program. Things to try include:
    a. Clicking and holding the mouse button then moving the cursor in order to rotate the molecule
    b. Checking the show bond angles box
    c. Checking the molecule geometry and electron geometry boxes
    d. Clicking on one of the atoms and moving it around to see the effect of this on the shape and how the bond angle responds
    e. Playing with the options to add and remove bonds and lone lone-pairs
3. Understand the basic geometries you need to be familiar with.
    a. Create a molecule in which a central atom is surrounded by 2 single bonds and no lone pairs
    b. Click and drag to have a good look at the three-dimensional shape
    c. Draw what you see (in three dimensions where relevant)
    d. Include the bond-angle on your diagram and the name of the molecule geometry
    e. Drag atoms around and look at how this affects the molecular shape and how the bond angles respond to this
    f. See if the geometry is affected by using double and triple bonds instead of single bonds
    g. Repeat with molecules with 3 and 4 single bonds (SL) or 3 to 6 single bonds (HL).
4. Now we will look at the shapes and bond-angles of some real-world molecules, some of which will seem not to follow the rules. Click on the 'Real Molecules' tab, we will be looking at: **HL only** - $SF_6$, $PCl_5$, $XeF_4$, $BrF_5$, $SF_4$; **HL and SL** – $CH_4$, $BF_3$, $CO_2$, $SO_2$, $NH_3$, $H_2O$. For each one:
    a. Click and drag to have a good look at the three-dimensional shape
    b. Draw what you see (in three dimensions where relevant)
    c. Include the bond-angle on your diagram and the name of the molecule geometry (and electron geometry)
    d. State whether the bond angles are as you would expect and where not, try to explain this difference.
    e. How do the model and real bond angles compare to each other? Can you explain this difference?

## Part 2: ACDLabs ChemSketch

1. Go to http://www.acdlabs.com/resources/freeware/chemsketch/ and follow the necessary steps to install ChemSketch.
2. Run ChemSketch
3. Have a play to familiarise yourself with the program. Include the following:
    a. Use the element symbols down the left-hand side to build up molecules – start with something simple like ethane.
    b. Select a molecule by dragging a box around it
    c. Exploring the Tools menu on a selected molecule. Tools of particular importance include 'Clean Structure', 'Add or Remove Explicit/Implicit Hydrogens', 'Generate' and 'Calculate'.
    d. Do a 'Save As…' and save the molecule as one of the two MDL Molfile options.
    e. Run the 3D Viewer program in the ACD Labs folder and open up the file you just saved.
    f. Click on the tetrahedral molecule icon towards the top-right of the screen to convert the image to 3D
    g. Play with the various options for displaying the molecule
    h. Use the bond angle tool to interrogate the structure
4. Draw some reasonably complicated molecules (10-20 atoms, C, H, N, O) in 3D format and predict the bond angles. Use the ChemSketch and 3D Viewer programs to model your molecule and check your predictions. **Note:** the program is not great at modelling lone pairs so it may be the program that is wrong sometimes rather than you!

# The Shapes of Molecules

| Electron Domains Around Central Atom | Example Compound(s) | Lewis Structure (showing bond angles, and in 3D where appropriate) | Bond Angle(s) (model and real) | Name of Shape |
|---|---|---|---|---|
| **2** ***(bonds only)*** | **$CO_2$** | | **Model:** **Real:** | |
| **3** ***(bonds only)*** | **$BF_3$** | | **Model:** **Real:** | |
| **3** **(2 bonds, 1 lone pair)** | **$SO_2$** | | **Model:** **Real:** | |
| **4** ***(bonds only)*** | **$CH_4$** | | **Model:** **Real:** | |
| **4** ***(1 lone pair, 3 bonds)*** | **$NH_3$** | | **Model:** **Real:** | |
| **4** ***(2 lone pairs, 2 bonds)*** | **$H_2O$** | | **Model:** **Real:** | |

| Electron Domains Around Central Atom | Example Compound(s) | Lewis Structure (showing bond angles, and in 3D where appropriate) | Bond Angle(s) (model and real) | Name of Shape |
|---|---|---|---|---|
| **5** ***(bonds only)*** | **$PCl_5$** | | **Model:** **Real:** | |
| **5** **(5 bonds, 1 lone pair)** | **$SF_4$** | | **Model:** **Real:** | |
| **6** ***(bonds only)*** | **$SF_6$** | | **Model:** **Real:** | |
| **6** **(5 bonds, 1 lone pair)** | **$BrF_5$** | | **Model:** **Real:** | |
| **6** ***(4 bonds, 2 lone pairs)*** | **$SF_6$** | | **Model:** **Real:** | |