**Determining Bond Angles Using Polygons**

**Bryce Dutcher – NSF Fellow Chemical Engineering Funded by: NSF GK-12**

**General description**

Bond angles of planar molecules are investigated. Basic concepts of polygon angle relationships are applied to calculate bond angles. These bond angles are then related to the stability of such molecules.

**Age group Estimated Time:** 55 minutes

**High School Geometry**

**Background**

In chemistry, a bond angle is the angle formed by two atoms bonded to another atom in any molecule. While most of molecules are three-dimensional, some molecules lie in two dimensions. When simple molecules exist in one plane, they can be represented by polygons. By making this simplification, it is easy to relate polygon angle relationships to determine the bond angles with little or no extra information. This provides the students one example of a practical use for polygon angle relationships.

**Concepts**

The primary concept introduced in this lesson is that of polygon angle relationships. Indirectly, students are exposed to molecular geometry and chemical stability.

**Vocabulary**

Molecule – two or more atoms bonded together

Bond Angle – angle formed by two atoms bonded to a third, central atom

Bond – electrons shared by two atoms which hold them together in a molecule

Double bond – formed when an atoms bonds to another atom twice

**Materials**

Molecular model kit (optional) for demonstrations

**Wyoming math standard**

MA 12.2.2

**Answer Key**

**Determining Bond Angles using Polygons**

In chemistry, a bond angle is the angle formed by two atoms bonded to another atom in any molecule. For example, a water molecule looks like this:

water.tif

An angle is formed by the bonds of each hydrogen atom (H) to the oxygen atom (O). In this particular example, the angle is 104.5°.

Let’s consider a simple molecule, borane (BH3). A single molecule of borane looks like this:

borane.tif

How many bond angles are formed in borane? Can you guess their value?

For borane, the answer may be obvious. There are three angles formed, all equal to 120°. One way to calculate this is to make each peripheral atom the point of a polygon. Adding line segments from each vertex through the central molecule allows us to visualize the bond angles. In symmetrical molecules, the central atom occupies the centroid of the resulting polygon. Borane, then, looks like a regular triangle, with boron at the centroid.

borane.tif

Now, using the angle relationships of a regular triangle, it can be proved that each bond angle is equal to 120°.

In the case of borane, we know the vertex angles must be 60° because it forms a regular triangle. When molecules do not exhibit such convenient symmetry, it is actually quite easy to measure the angle of each vertex in a laboratory based on the size of the molecule. In this manner, we can in theory determine the bond angles of any planar molecule.

Let’s consider fluoroborane (BH2F), which looks like this:

fluoroborane.tif

Notice that a fluorine atom is larger than a hydrogen atom. How do you think this might affect the geometry of the molecule?

Larger molecules force other molecules away from then, so the H-B-H bond will be compressed slightly.

Based on experimental data, what are the values of the three bonds angles of fluorborane?

∠BAC = ∠ACB = 61.3°

∠ACD = 32.5°

∠ADC = 115°

∠ADB = 122.5°

∠BDC = 122.5°

fluoroborane.tif

D

C

B

A

Here are a few more possible molecular geometries. Based on the given data, see if you can determine the value of the bond angles. Note: Images are not necessarily drawn to scale.

∠BAC = ∠ACD =60°

∠CAD = 40.9°

∠CBD = 16.1°

∠ADC =79.1°

∠ADB =147°

∠BDC =133.9°

A

C

B

D

‖

∠BAD = 70° ∠AEB = 70°

∠ABC = 80° ∠BEC = 110°

∠ADB = 60° ∠CED = 70°

∠ACB= 40° ∠AED = 110°

C

E

D

A

B

∠ABC = ∠AED = 80°

∠BCD = ∠CDE = 120°

∠AEF= 45°

∠DCF= 70°

∠AFB = 65°

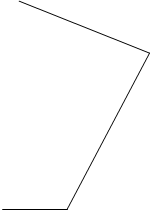
∠BFC = 95°

∠CFD = 40°

∠DFE = 95°

∠AFE = 65°

A



F

E

D

C

B

Can you guess why knowing the value of bond angles is important?

It relates to stability.

Let consider a carbon bonded to two other carbons and a hydrogen. Strictly speaking, this is not a molecule, but a unit that can be part of a larger molecule. It looks like this:

Carbon unit.tif

Based on our analysis of borane and fluorborane above, can you guess the value of the C-C-C bond angle?

We would expect the C-C-C bond to be larger than 120°, and the two C-C-H bonds to be smaller than 120°. In reality, however, they are all very close to 120° due in large part to the double bond.

Despite the size difference of the carbon and hydrogen atoms, this triangular arrangement of carbon is most stable at 120°.

To illustrate this, let’s consider three ring-type molecules.:

cylclopropene.tifbenzene.tifcyclooctene.tif

Cyclopentene Benzene Cyclooctene

Which of these molecules is most stable? Why?

Benzene, since the interior angles of a regular hexagon are 120°, equal to the stable bond angle of carbons.

Can you guess which of these is the least stable? Why would you guess so?

Cyclopentene is actually the least stable due to the very high strain of the compressed bond (the interior angles of a regular triangle are 60°, farther away from the stable 120° than the 135° of a regular octagon). This molecule explodes easily.

**Student Worksheet**

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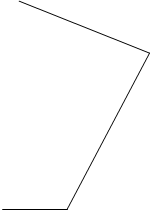
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