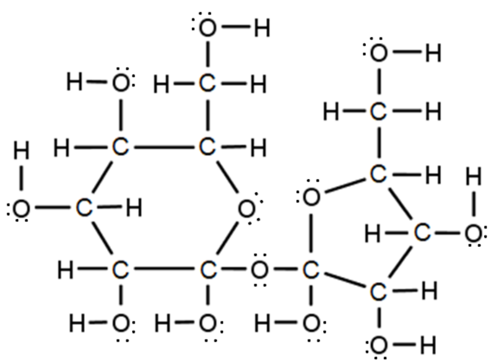
Learning Guide Module

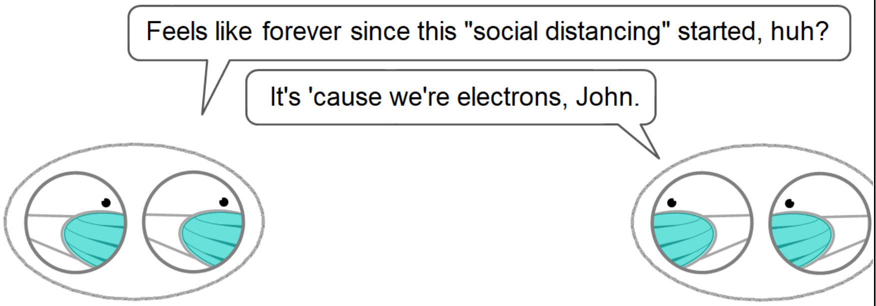
Subject Code	Chemistry 1	General Inorganic Chemistry 1
Module Code	4.0	Chemical Bonding
Lesson Code	4.4	Molecular Geometry
Time Limit		30 minutes

Components	Tasks	TA[a]	ATA[b]
Target 	By the end of this module, the students will have been able to: 1. Identify the electron domain geometries and molecular geometries 2. Predict the structures of molecules and polyatomic ions using the Valence Shell Electron Pair Repulsion (VSEPR) Theory	1 min	
Hook 	A molecule of *sucrose*, commonly known as table sugar, owes its sweet taste to its three-dimensional structure. Unfortunately, we cannot visualize this from its two-dimensional Lewis representation.  Lewis structure of sucrose How different is a real sucrose molecule from the Lewis representation above? Are bonds and lone pairs in the actual molecule positioned arbitrarily, or are they arranged in a specific way? To get a glimpse of how structure is related to sweetness, you may watch the video *Why Do Things Taste Sweet?*[1] and skip to 0:44 – 2:18. (If you do not have access to the video, read the transcript provided at the end of this learning guide.)	3 min	

Ignite

10 min

Molecules and polyatomic ions consist of electron pairs found in *covalent bonds* and (oftentimes) in *lone pairs*. These negatively charged bonds and lone pairs in a molecule experience repulsion, similar to how the like poles of two magnets repel each other. For this reason, electron pairs arrange themselves in a way that they are farthest apart to minimize repulsion forces.

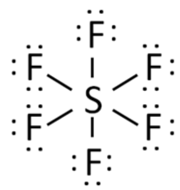


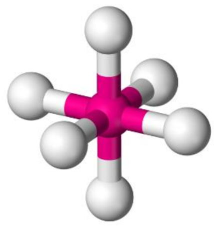
I. <u>Can Lewis structures tell us a molecule's shape?</u>

Using Lewis structures is a practical way of representing molecules and polyatomic ions, but these cannot show the accurate positions of bonds in three dimensional space. For example, the Lewis structure of sulfur hexafluoride (SF_6) cannot depict F atoms positioned at 90° angles around S.

► COMPARISON

The Lewis structure of SF_6 is shaped like an asterisk. Its real shape is similar to that of a jackstone.



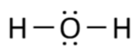
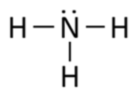
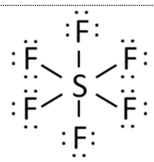
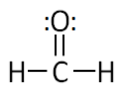


Actual shapes of molecules and polyatomic ions are determined through experiment; however, as you read on, we will learn that there is a faster and easier way. We will explore a theory that allows us to predict shapes just by looking at Lewis structures.

The **Valence-Shell Electron-Pair Repulsion (VSEPR) theory** states that shapes of molecules and polyatomic ions depend on the **number of electron domains** around a **central atom**. An *electron domain* can refer to a bond or a lone pair. Water has two H atoms bonded to the central atom O, which has two lone pairs around it. This means that O has a total of four electron domains. (<u>Note</u>: A double bond or a triple bond is counted as one electron domain only, similar to a single bond.)

AXE notation is often used to write a generic formula describing the electron domains around a central atom, **A**. The subscript of **X** denotes the number of *atoms* bonded to A, while the subscript of **E** denotes the number of *lone pairs* around A. The AXE notation of water, or H_2O, is expressed as AX_2E_2.

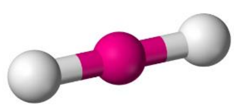
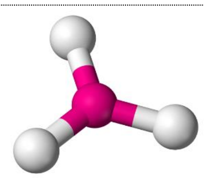
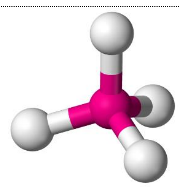
Before we proceed with electron domain geometries, try filling out this table:

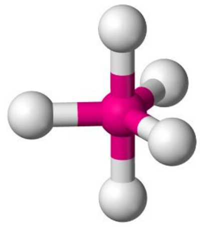
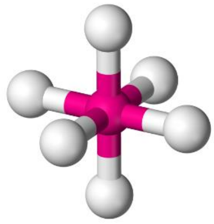
Lewis structure				
Central atom (A)	O (oxygen)			
No. of atoms bonded to A (X)	2			
No. of lone pairs around A (E)	2			
No. of electron domains around A	4			
AXE notation	AX_2E_2			

(Answers: NH_3 – N, 3, 1, 4, AX_3E; SF_6 – S, 6, 0, 6, AX_6; CH_2O – C, 3, 0, AX_3)

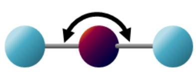
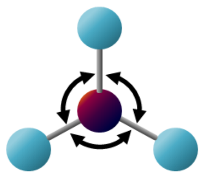
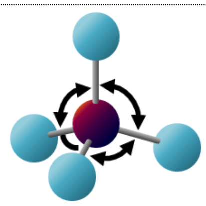
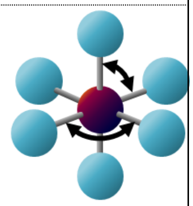
II. What is electron domain geometry?

Electron domain geometry shows how electron domains are arranged in a specific way around a central atom. The most common electron domain geometries are as follows:

		
Linear 2 electron domains (sp hybridization)	Trigonal planar 3 electron domains (sp^2 hybridization)	Tetrahedral 4 electron domains (sp^3 hybridization)

	
Trigonal bipyramidal 5 electron domains (sp^3d hybridization)	Octahedral 6 electron domains (sp^3d^2 hybridization)

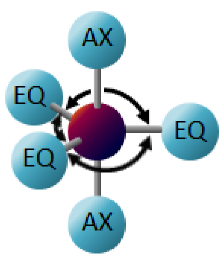
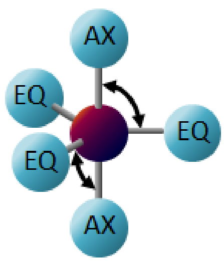
Each geometry has ideal bond angles. The bond angles are 180°, 120°, 109.5°, and 90° in linear, trigonal planar, tetrahedral, and octahedral geometries, respectively.

Linear	Trigonal planar	Tetrahedral	Octahedral
180° 	 120° all angles	 109.5° all angles	 90° all angles

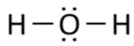
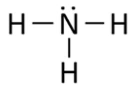
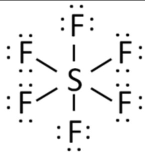
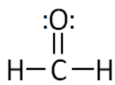
Trigonal bipyramidal geometry has two bond angles. Equatorial bonds, as show in the diagram below, are 120° apart. Axial bonds are perpendicular (90°) to the equatorial bonds.

► TRIGONAL BIPYRAMIDAL

You may notice that this geometry looks like a combination of linear and trigonal planar geometries.

	
120° between equatorial (EQ) bonds	90° between EQ and axial (AX) bonds

Going back to H_2O as our example, the four (4) electron domains around oxygen indicate that its electron domain geometry is tetrahedral. Try matching each molecule with its correct electron domain geometry to fill out the table:

Lewis structure				
EDG	tetrahedral			

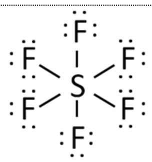
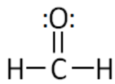
(Answers: NH_3 – tetrahedral; SF_6 – octahedral; CH_2O – trigonal planar)

III. What is molecular geometry?

In contrast to electron domain geometry (EDG), **molecular geometry** (MG) distinguishes bonds from lone pairs. In particular, molecular geometry shows the arrangement of bonded atoms only. When referring to a simple molecule's *shape*, molecular geometry is usually used.

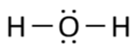
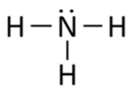
► NO LONE PAIRS

If the central atom has no lone pairs, its EDG would be the same as its MG.

	
AX_6 EDG: Octahedral MG: Octahedral	AX_3 EDG: Trigonal planar MG: Trigonal planar

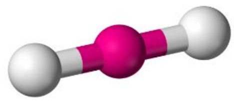
► WITH LONE PAIRS

MG varies depending on the number of bonds and number of lone pairs. Can you identify the MG of H_2O and NH_3? Read on to know the answer.

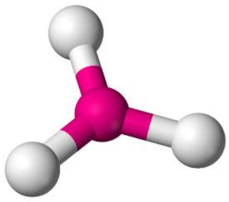
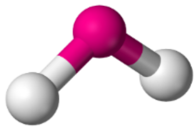
	
AX_2E_2 EDG: Tetrahedral MG: ____________	AX_3E EDG: Tetrahedral MG: ____________

The following are the fifteen molecular geometries grouped according to the number of electron domains.

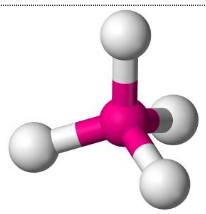
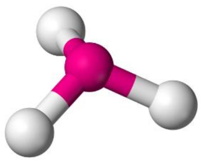
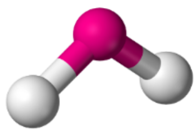
Linear (2 electron domains)**:**


AX_2 Linear

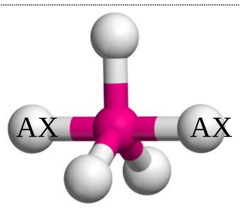
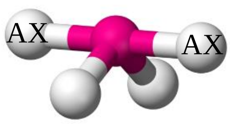
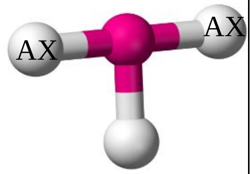
Trigonal planar family (3 electron domains)**:**

	
AX_3 Trigonal planar	AX_2E Bent

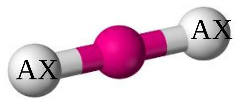
Tetrahedral family (4 electron domains)**:**

		
AX_4 Tetrahedral	AX_3E Trigonal pyramidal	AX_2E_2 Bent

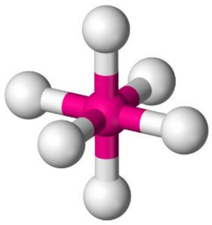
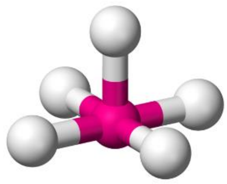
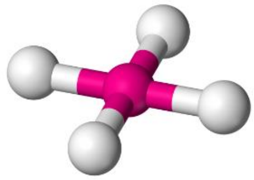
Trigonal bipyramidal family (5 electron domains)**:**

		
AX_5	AX_4E	AX_3E_2

Trigonal bipyramidal	See-saw	T-shape


AX_2E_3 Linear

Octahedral family (6 electron domains)**:**

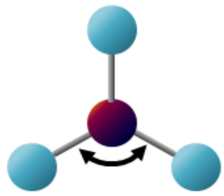
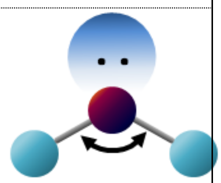
		
AX_6 Octahedral	AX_5E Square pyramidal	AX_4E_2 Square planar

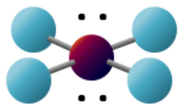
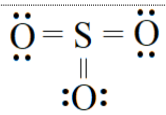
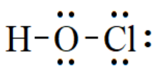
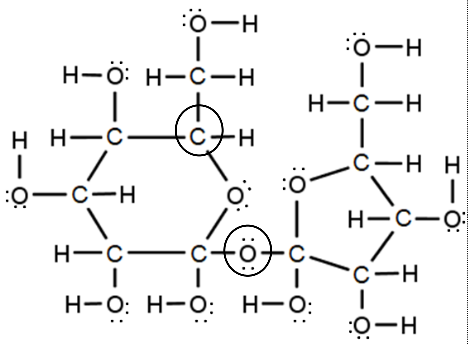
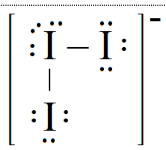
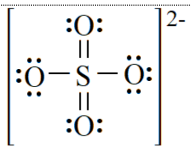
IV. When do bond angles deviate from ideal?

Bonds experience stronger repulsion from lone pairs than from other bonds. Actual bond angles differ slightly from the ideal values because of this.

► SMALLER BOND ANGLES

Lone pairs take up more space due of stronger repulsion. In turn, bonds are “compressed” and the bond angle between them becomes less than the ideal.

 Exactly 120^o	 Less than 120^o

	▶ LINEAR AND SQUARE PYRAMIDAL Though lone pairs distort bond angles, linear (AX_2E_3) and square planar (AX_4E_2) are exceptions. The symmetry in each MG cancels out the effect of lone pairs.  Exactly 180°  Exactly 90°		
Navigate	Let's test what you've learned! A. Answer questions 1-4 on your own. These will not be graded. For numbers 1-2, refer to the given Lewis structures:      1. Give the AXE notation, electron domain geometry, and molecular domain geometry of: a. Sulfur trioxide (SO_3) b. Hypochlorous acid (HOCl) c. Triiodide ion (I_3^-) d. Sulfate ion (SO_4^{2-}) e. Encircled C atom in sucrose f. Encircled O atom in sucrose 2. Compare bond angles by writing the symbols < , > , or =. a. ∠OSO in sulfur trioxide ______ ∠OSO in sulfate b. ∠HOCl in hypochlorous acid ______ ∠III in triiodide c. ∠CCC in sucrose ______ ∠COC in sucrose	15 min	

3. Challenge: Give the molecular geometry of each hypothetical compound. Make sure to draw Lewis structures first to get the answer.
   a. SeH_4 b. SBr_3^+ c. TeI_5^-

B. Fill out the table by giving the correct information for each hypothetical compound. This activity will be graded. Email your teacher a photo or scanned copy of your answers.

	$ArBr_2$	AsH_3^{2-}
Lewis structure	1.	6.
AXE notation	2.	7.
EDG	3.	8.
MG	4.	9.
Bond angles (state whether it is exact or approximate)	5.	10.

Knot 	In summary: • The valence-shell electron-pair repulsion (VSEPR) theory predicts the arrangement of electron domains around a central atom. • Electron domain geometry (EDG) is determined by the number of electron domains. It does not distinguish bonds from lone pairs. • Molecular geometry (MG) is determined by the number of bonds and number of lone pairs. This describes the “shape” of a molecule, or the arrangement of bonded atoms around a central atom. • A bond angle is the angle between two adjacent bonds in a molecule or polyatomic ion. Bond angles become smaller than their ideal values when a lone pair is present because of greater repulsion.	1 min	

[a] suggested time allocation set by the teacher
[b] actual time spent by the student (for information purposes only)

Endnotes:
(1) Video produced by the American Chemical Society. Published in “Reactions” Youtube channel on October 21, 2014.

References:
American Chemical Society (October 21, 2014). Why Do Things Taste Sweet. https://www.youtube.com/watch?v=FaBFyEa8-el

Burdge, J. and Overby, J. (2012). Chemistry: Atoms First (1st ed.). United States of America: McGraw Hill.

Silberberg, M. (2008). Chemistry: The Molecular Nature of Matter and Change (5th ed.). United States of America: McGraw Hill.

Prepared by: Arianne A. Won
Position: Special Science Teacher (SST) II
Campus: PSHS-MC

Reviewed by: Lester Mendoza
Position: Special Science Teacher (SST) II
Campus: PSHS-MC