8.13 - Molecular Shape

Shape Overview

Previously you learned how individual bonds have particular characters based on electronegativity differences.

Next you saw how Lewis structures can be made based on the octet rule, and formal charge considerations.

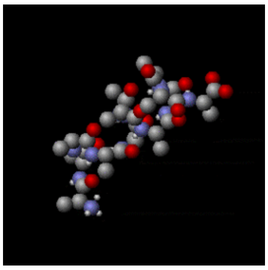
Here, you will learn how Lewis structures relate to the actual configuration of a molecule in 3-D space, and will be able to predict whether a molecule will be polar or not.

VSEPR Model

When predicting the shapes of molecules, it's important to remember that electrons repel other electrons due to electrostatic interactions.

The Valence Shell Electron Pair Repulsion (VSEPR) model predicts shapes of molecules, by treating bonded and non-bonded pairs of electrons as mutual repellers trying to push each other as far away as possible.

Wiggly Molecule!



Hybridization

Hybrid: two things combine, forming something with characteristics of both.

Hybridized orbitals occur when atomic orbitals (s, p, and d) mix, & form new, symmetric orbitals.

The hybridization of the **central atom** determines shape.

Determining Hybridization & Shape

0. Make a Lewis structure of your molecule.

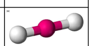
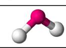
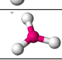
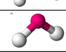
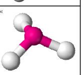
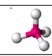
1. Add lone pairs & terminal atoms for the CENTRAL ATOM only. You should get a number from 1 - 6.

2. Determine hybridization of central atom:

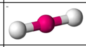
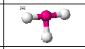
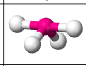
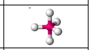
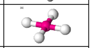
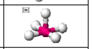
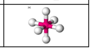
1 = s	2 = sp	3 = sp^2
4 = sp^3	5 = sp^3d	6 = sp^3d^2

3. Using the Molecular Shapes Resource, determine shape (Using lone pair count, number of terminal atoms, and hybridization).

Molecular Shapes Resource Page 1

Molecular Shape	Ex.	Terminal Atoms	Lone Pairs	Hybrid-ization	Angles	Molecular Appearance
Linear Diatomic (2 atoms)	HCl	1	NA	s	NA	
Linear	CO2	2	0	sp	180º	
Bent	O3	2	1	sp2	120º	
Trigonal Planar	BH3	3	0	sp2	120º	
Bent	H2O	2	2	sp3	104.5º	
Trigonal Pyramidal	PH3	3	1	sp3	107.3º	
Tetrahedral	CH4	4	0	sp3	109.5º	

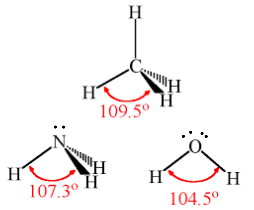
Molecular Shapes Resource Page 2

Molecular Shape	Ex.	Terminal Atoms	Lone Pairs	Hybrid-ization	Angles	Molecular Appearance
Linear	XeF_2	2	3	sp^3d	180°	
T – Shaped	ClF3	3	2	sp3d	180o 90o	
Seesaw	SF_4	4	1	sp3d	180o 120o 90o	
Trigonal Bipyramidal	TeF_5	5	0	sp3d	120º 90º	
Square Planar	XeF4	4	2	sp3d2	180o 90o	
Square Pyramidal	BrF5	5	1	sp3d2	180o 90o	
Octahedral	SF6	6	0	sp3d2	90º	

Bond Angle

Bond Angle is the angle between a central atom and its terminal atoms.

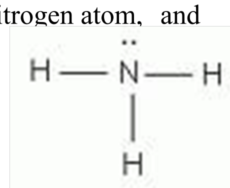
While the exact details of bond angle rely to some extent on which atoms are the terminal atoms, it is geometrically possible to post approximate bond angles (as are in the resource).



1. Shape of Ammonia Example

What is the hybridization of the nitrogen atom, and overall shape of ammonia (NH_3)?

First, figure out Lewis structure:



Terminal atoms = 3

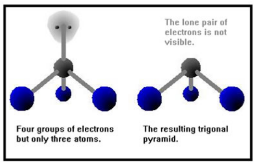
Lone pairs = 1

Hybridization = sp^3

What shape is it?

Trigonal pyramidal

(Model Demo).

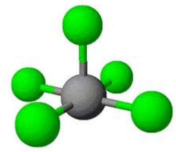


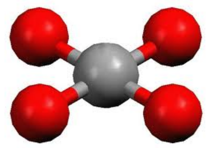
Bond angle = 107.3°.

Expanded Octet

Central atoms can have more than 8 electrons.

D orbitals are involved, and leads to sp^3d or sp^3d^2 hybridization.

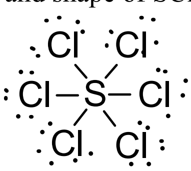




2. Expanded Example

What's the hybridization and shape of SCl_6?

Lewis Structure:



Terminal Atoms = 6

Lone Pairs = 0

Hybridization = sp^3d^2

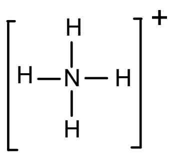
Shape = Octahedral

Bond angle = 90°.

3. Ammonium Ion Example

What's the hybridization and shape of NH_4^+?

Lewis Structure:



Terminal atoms = 4

Lone pairs = 0

Hybridization = sp^3

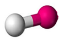
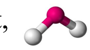
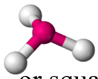
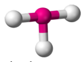
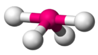
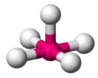
Shape = Tetrahedral

Determining Polarity Process

Two things determine polarity:

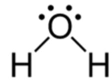
1. Absolute electronegativity difference between central and at least one terminal atom must be between 0.4 and 1.9.

2. Make Lewis structure; molecule must be asymmetric, either by:

A. shape: linear diatomic,  bent,  trigonal pyramidal,  t-shaped,  seesaw,  or square pyramidal; 

B. OR composition: different terminal atoms.

4. Is H_2O Polar?

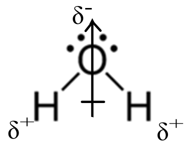


What is the electronegativity difference?

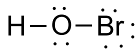
Oxygen - hydrogen:
3.5 - 2.1 = 1.4: polar covalent bond.

What's the shape?

H_2O is bent (asymmetric), so it is polar.

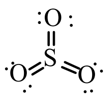


Guided Practice: Polar or not?

5. HOBr 

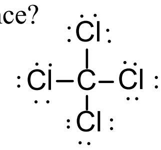
Electronegativity Differences:
H vs O = 1.4; Br vs. O = 0.7: Could be polar

Shape: Bent: It's Polar

6. SO_3 

Electro. difference:
S vs. O = 1.0: Could be polar.
Shape: Trig. Planar: Not Polar

7. Is CCl_4 Polar?

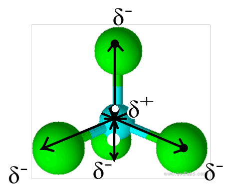


What is the electronegativity difference?

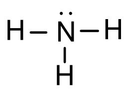
Chlorine - carbon:
3.0 - 2.5 = 0.5: polar covalent bond.

What's the shape?

CCl_4 is tetrahedral with same terminal atoms: it is non-polar.



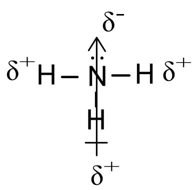
8. Is Ammonia (NH_3) Polar?



Are there polar bonds?
What's the shape?

Electronegativity difference:
nitrogen - hydrogen
3.0 - 2.1 = 0.9: polar covalent bonds.

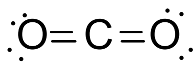
Shape is trigonal pyramidal: it is polar.



9. CO_2 Example!

Is carbon dioxide polar?

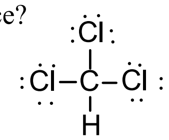
Electronegativity difference:
oxygen - carbon: 3.5 - 2.5 = 1.0: polar covalent.

Shape? 

The shape is linear: non-polar.

10. Is $CHCl_3$ Polar?

What is the electronegativity difference?



Chlorine - carbon:
3.0 - 2.5 = 0.5: polar covalent bond.
Hydrogen - carbon:
2.1 - 2.5 = non-polar bond

What's the shape?

$CHCl_3$ is tetrahedral with different terminal atoms: it is polar.

Homework

8.13 Problems in your Booklet
Due: Next Class

Finish 6.B Review Scan Problems:
Due Friday, 3/6