CHM 101
GENERAL CHEMISTRY 1

HYBRIDIZATION AND SHAPES OF MOLECULES

By

DR. OLUBUNMI A. ADEWUSI
Department of Chemistry,
Lagos State University, Ojo, Lagos

LEARNING OBJECTIVES

- **Know what sigma and pi bonds are, and examples of simple molecules having them.**
- **Understand sp^2, and sp^3 orbital hybridization with specific examples.**
- **Understand the principles of the valence shell electron pair repulsion (VSEPR) theory used in the prediction and the interpretation of shapes/geometry of simple molecules and ions.**
- **Understanding of the term bond angle.**
- **Know the shapes/geometry and bond angles of $BeCl_2$, BCl_3, CH_4, NH_3, H_2O, CO_2, PCl_5, SF_6 and C_2H_4.**
- **Be able to use VSEPR to predict shapes/geometry, bond angles of similar molecules to the ones given above.**

SIGMA (σ) BOND

Sigma bonds are the strongest type of covalent bonds due to the direct overlap of valence orbitals, and the electrons in these bonds are sometimes referred to as sigma electrons. A single bond is usually a sigma bond.

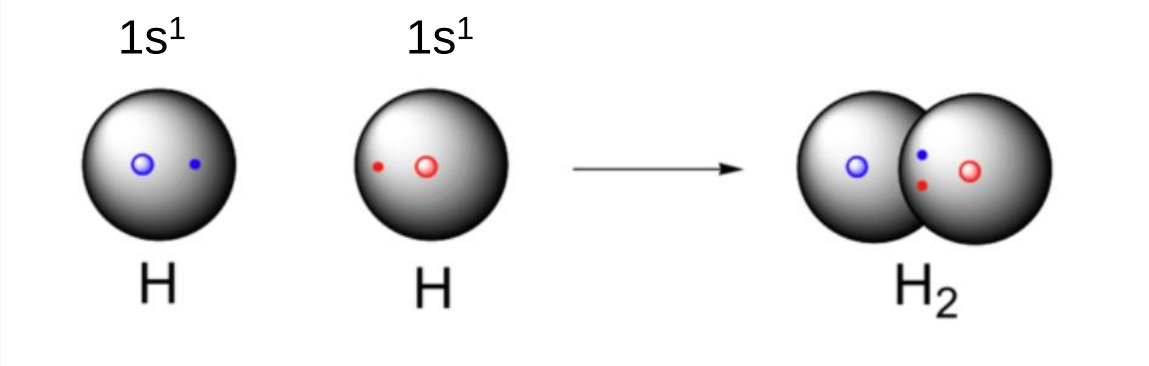
ONE

HYDROGEN (H_2)

The simplest molecule to use to explain is the hydrogen molecule.

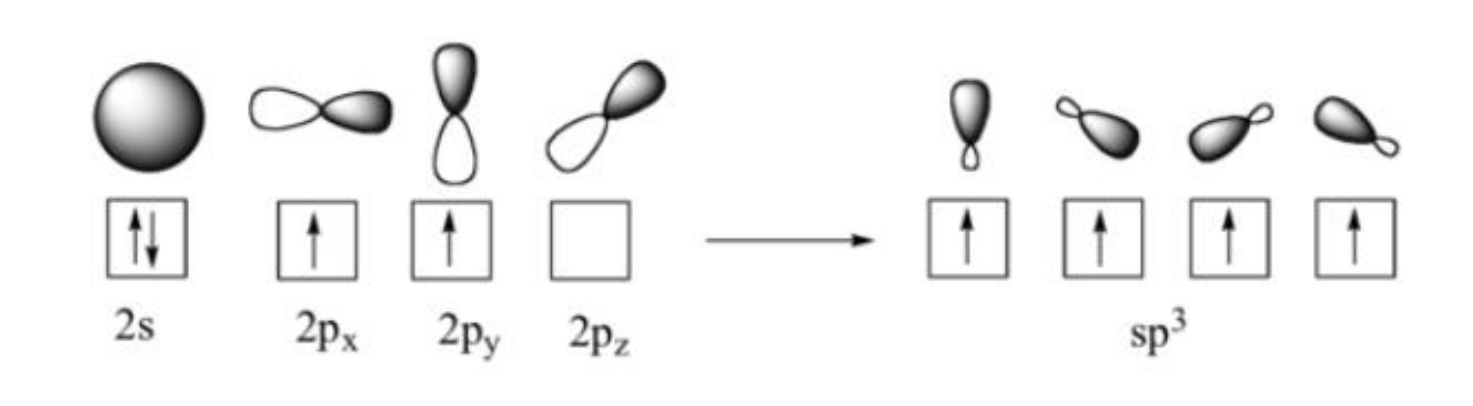
Each atoms provides a 1s electron which is used in covalent bonding through the overlap of the two 1s orbitals, hence forming a pair within the two overlapping orbitals

The two electrons forms a strong bond like a glue because of the strong attraction they experience to the positive nuclei of the atoms



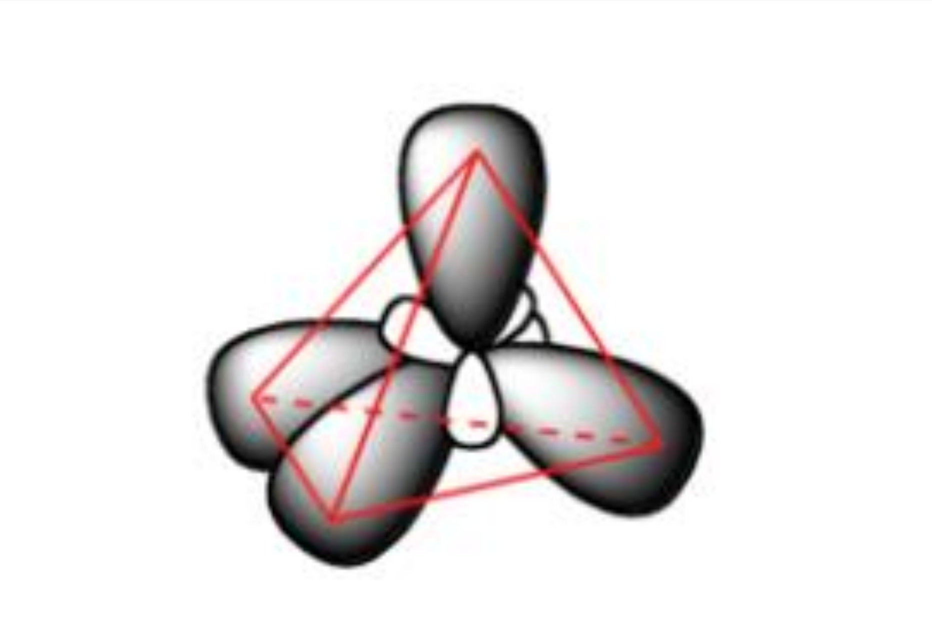
example

TWO

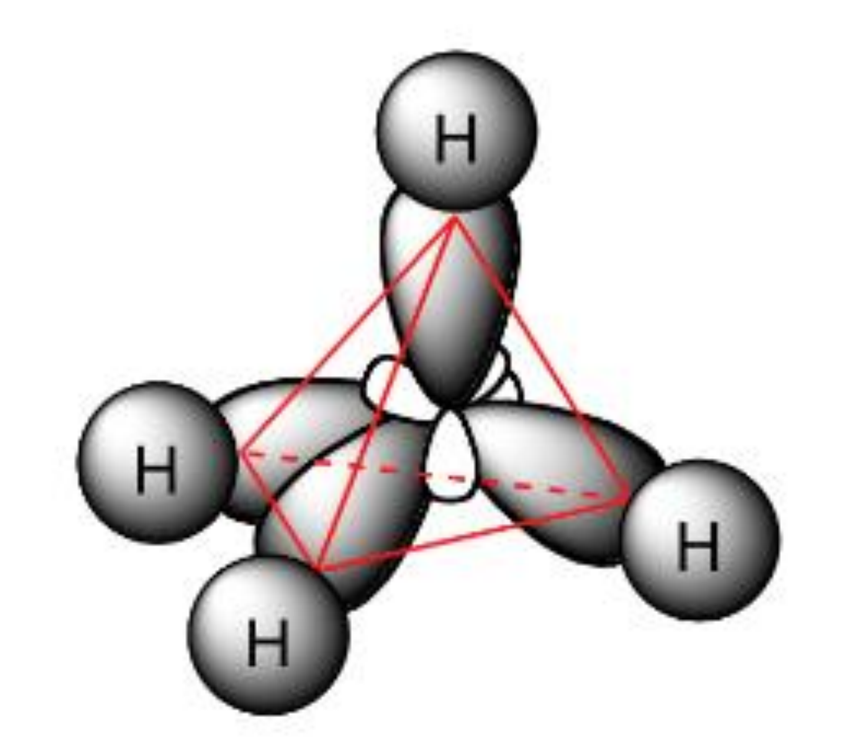


METHANE (CH_4)

- ✓ The simplest organic molecule
- ✓ Carbon $1s^2, 2s^2, 2p_x^{\ 1}, 2p_y^{\ 1}, 2p_z$
- ✓ A concept called orbital hybridization takes place for the carbon atom to be able to have a single bond each with the four hydrogen atoms. This is explained by valence bond theory (VBT)
- ✓ The four valence orbitals of the carbon (one 2*s* and three 2*p* orbitals) combines to form four equivalent hybrid sp^3 orbitals because they are formed from mixing one s and three p orbitals. In the new electron configuration, each of the four valence electrons on the carbon occupies a single sp^3 orbital.
- ✓ The four C-H bonds in methane are arranged with tetrahedral geometry about the central carbon, with each bond hav the same length and strength.
- ✓ The sp^3 hybrid orbitals are oblong in shape similar to the *p* orbitals of which they are partly made up of with two lobes of opposite sign but the two lobes have different sizes unlike the regular p orbital. The bigger lobes are directed towards the four corners of a tetrahedron, making the angle between any two orbital in methane to be 109.5^{o}.



sp^3 hybridized carbon

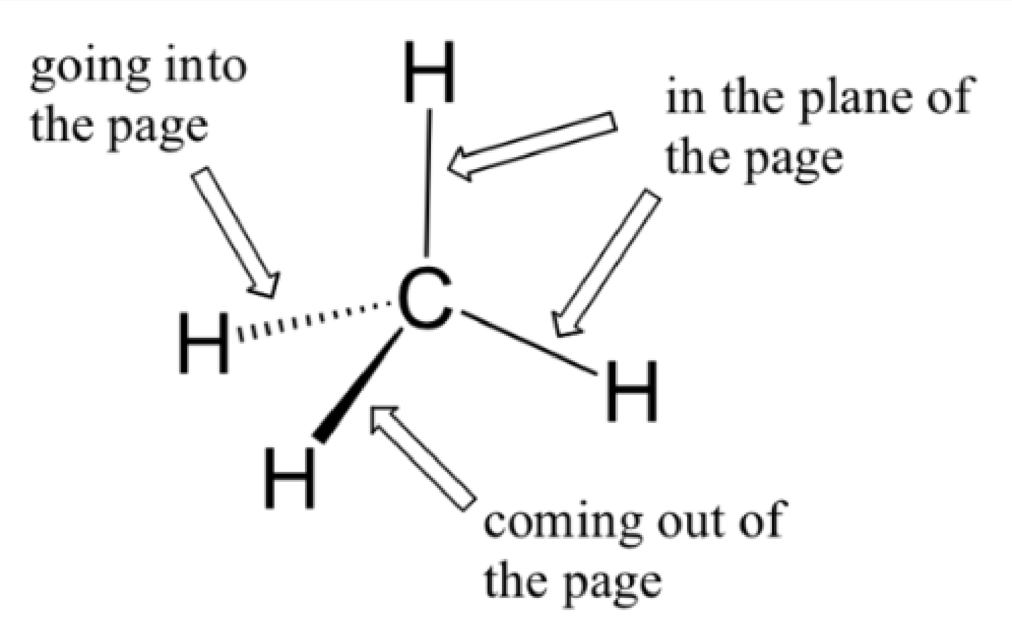


sp^3 hybridized carbon bonded to four hydrogen atoms

- ✓ **The four C-H bonds in methane are of equal length of 1.09 Å (1.09×10^{-10}m). Each is formed from the overlap between a half-filled 1*s* orbital in a hydrogen atom and a sp^3 hybrid orbital in the central carbon.**

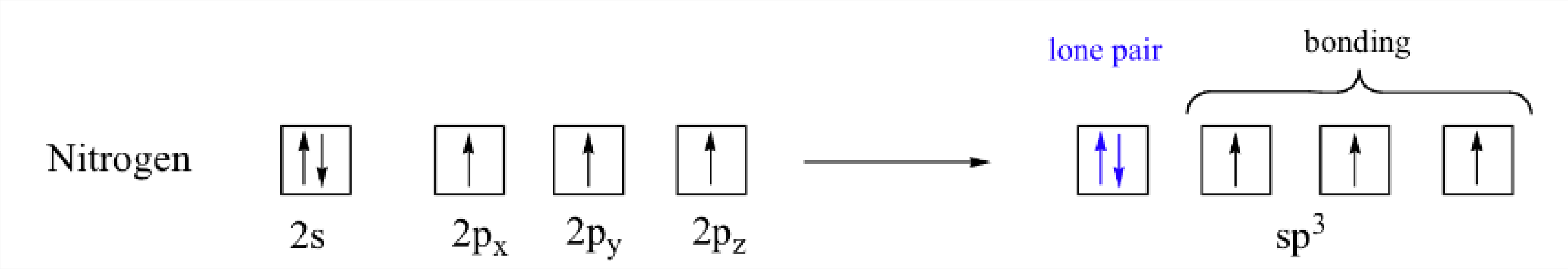
THE SOLID DASH/WEDGE SYSTEM

It is a conventional way of drawing 2-dimentional structures of molecules. A solid wedge simply represents a bond that is meant to be pictured emerging from the plane of the page. A dashed wedge represents a bond that is meant to be pictured pointing into, or behind, the plane of the page. Normal lines imply bonds that lie in the plane of the page.



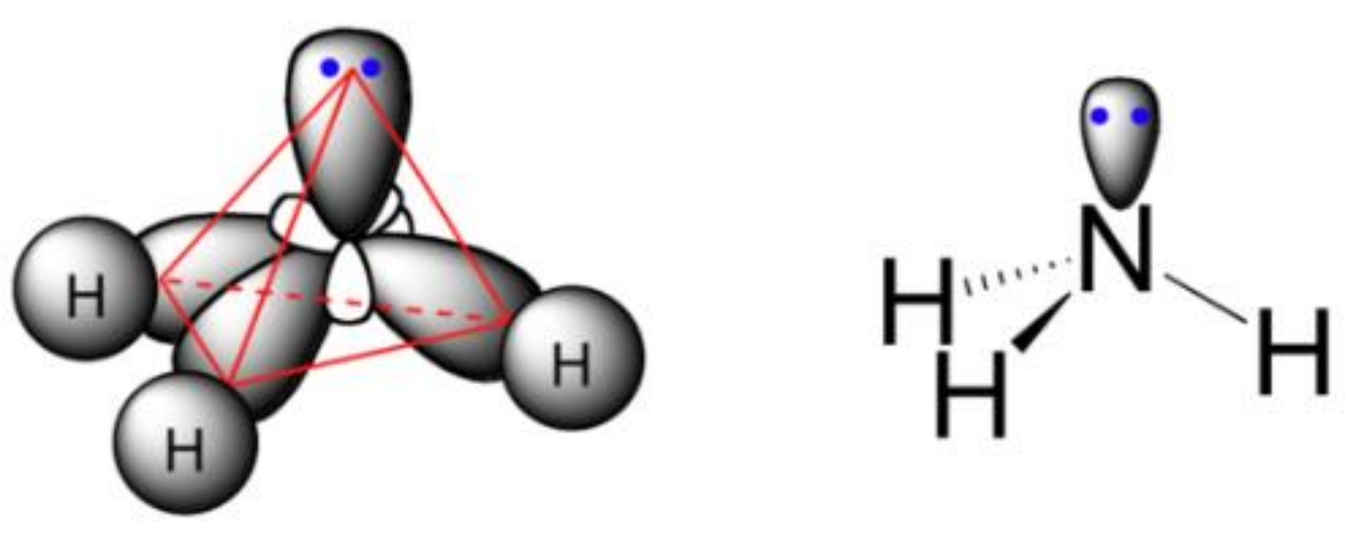
example

THREE



AMMONIA (NH_3)

- ✓ **Nitrogen is sp^3 hybridized.**
- ✓ **The bonding arrangement is also tetrahedral where the three N-H bonds of ammonia forms the base of a trigonal pyramid. The fourth orbital which has the lone pair forms the top of the pyramid.**
- ✓ **The lone pair due to its slightly greater repulsive effect pushes the three N-H bonds away from the top of the pyramid, making the H-N-H bond angles not to tetrahedral at 107.3˚.**



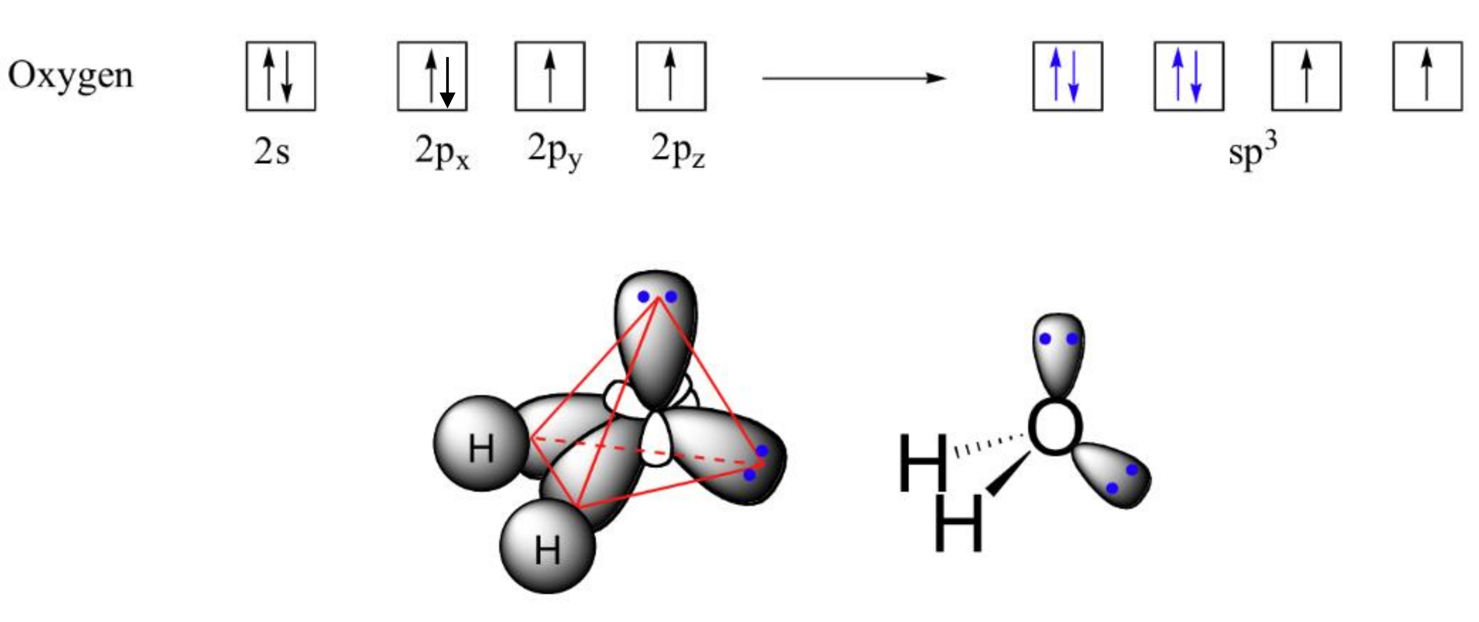
example

FOUR

WATER (H_2O)

- ✓ The overlap of sp^3 hybrid orbitals on oxygen with 1s orbitals on the two hydrogen atoms makes the bonding in water to occur.

- ✓ The two nonbonding lone pairs on oxygen would be located in sp^3 orbitals. A molecule of water molecule is ‘bent’ at an angle of approximately 104.5˚(explained by VSERP).



pi (π) BONDS

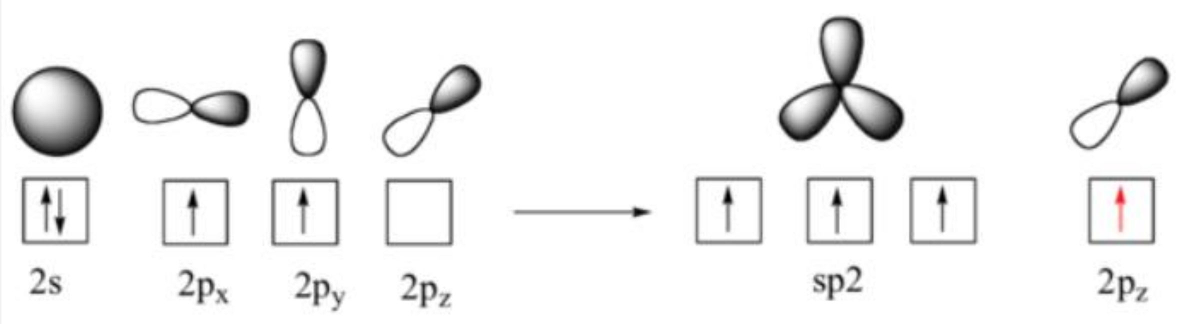
sp^2 hybridization

FIVE

ETHENE C_2H_2

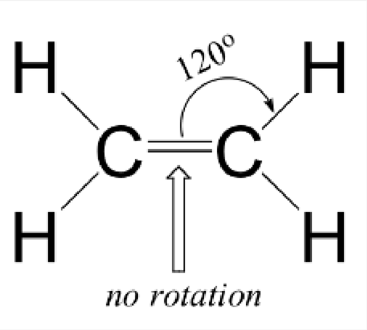
Valence bond theory, and the hybrid orbital concept, describes bonding in double-bonded compounds like ethene.

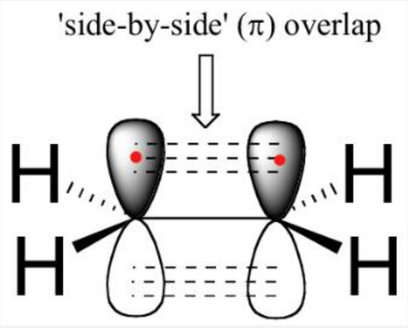
- ✓ The 2*s*, 2p_x and 2p_y orbitals combine to form three sp^2 hybrid orbitals, leaving the 2p_z orbital unhybridized.



Characteristics of the ethene molecule relating to its bonding.

- ✓ It is a planar (flat) molecule.
- ✓ Bond angles are approximately 120 º, and the C-C bond length is 1.34 Å, significantly shorter than the 1.54 Å single carbon-carbon bond in ethane.
- ✓ There is no rotation about the carbon-carbon double bond.





The valence shell electron pair repulsion (VSEPR) theory

ELECTRON PAIR REPULSION THEORY

The **electron pair repulsion (EPR) theory** states that:

- the shape of a molecule or ion is caused by repulsion between the pairs of electrons, both bond pairs and lone (non-bonding) pairs, that surround the central atom
- the electron pairs arrange themselves around the central atom so that the repulsion between them is at a minimum
- lone pair–lone pair repulsion > lone pair–bond pair repulsion > bond pair–bond pair repulsion.

LEARNING TIP

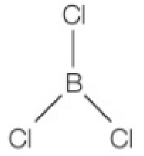
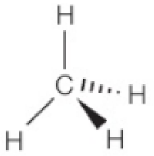
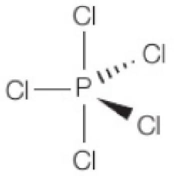
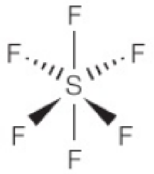
This theory is sometimes also called the valence shell electron pair repulsion theory, abbreviated to VSEPR.

The first two rules are used to obtain the basic shape of the molecule or ion. The third rule is used to estimate values for the bond angles.

THE SHAPES OF MOLECULES AND IONS

To obtain the shape of a molecule or ion it is first necessary to obtain the number of bond pairs and lone pairs of electrons around the central atom.

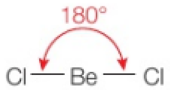
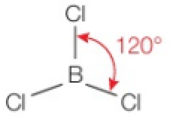
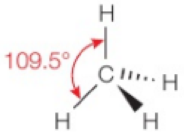
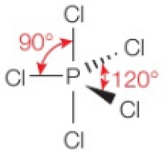
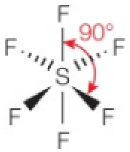
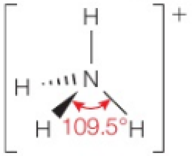
More Examples

NUMBER OF BOND PAIRS	NUMBER OF LONE PAIRS	SHAPE	EXAMPLE
2	0	linear	Cl — Be — Cl
3	0	trigonal planar	
4	0	tetrahedral	
5	0	trigonal bipyramidal	
6	0	octahedral	
3	1	trigonal pyramidal	
2	2	V-shaped	

Shapes of molecules.

THE BOND ANGLES IN MOLECULES AND IONS

Table B shows the bond angles of a range of molecules and ions.

Linear, e.g. $BeCl_2$ The bond angle is 180°. 	Trigonal planar, e.g. BCl_3 The bond angle is 120°. 
Tetrahedral, e.g. CH_4 The bond angle is 109.5°. 	Trigonal pyramidal, e.g. NH_3 The bond angle is 107°.  Lone pair–bond pair repulsion is greater than bond pair–bond pair repulsion, so the angle is slightly less than 109.5°.
V-shaped, e.g. H_2O The bond angle is 104.5°.  Lone pair–lone pair repulsion is greater than lone pair–bond pair repulsion, so the bond angle is even further depressed from 109.5°, and is slightly less than the 107° in NH_3.	Trigonal bipyramidal, e.g. PCl_5 There are two bond angles: 90° and 120°. 
Octahedral, e.g. SF_6 There are two bond angles: 90° and 180°.  The angle between the bonds of two fluorine atoms opposite one another is 180°.	Tetrahedral, e.g. NH_4^+ As with CH_4, the bond angles are 109.5°.  Note the change from 107° in ammonia to 109.5° in the ammonium ion.

The bond angles of a range of molecules and ions.

REFERENCES

1. Pearson-International. A-Level-Chemistry

2. Education-career. Online image from https://www.apa.org/ on June 6, 2023.

3. Chem.libretexts.org. Structure and Properties of Organic Molecules. Hybridization and Molecular Shapes (Review). Online excerpt on June 6, 2023.