Kegn Andarge Welde-Giorgis Memorial school
2012; Grade 11, Chemistry.

Molecular Geometry

Valence Shell Electron Pair Repulsion Theory (VSEPR)

* The basic principle of VSEPR theory: 'pairs of valence electrons around the central atom stay as far apart as possible from each other to minimize repulsions among them.'

Electron Arrangement and Molecular Shape

→ The electron pair arrangement is defined by the sets of electrons, both bonding and non-bonding (lone pair) around the central atom.

→ The molecular shape is defined by the relative positions of the atomic nuclei in the molecule.

→ To classify molecular shapes, the AX_mE_n designation is assigned, where A is the central atom, X is the terminal atom, E is lone pair m and n are positive integers. The arrangements that best minimize repulsions naturally depend on the number of electron sets.

→ Order of repulsions: Lone Pair – Lone Pair > Lone Pair Bond Pair > Bond Pair – Bond Pair

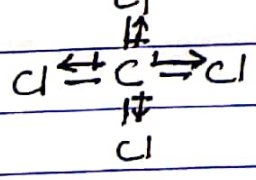
→ All molecules have shapes that can be considered to be derived from basic sets of five different geometries:
Linear, Trigonal Planar, Tetrahedral, Trigonal Bipyramidal and Octahedral.

Molecular Shape and Molecular Polarity

→ Molecular polarity is created by molecules with a net imbalance of charge. In molecules with more than two atoms, both shape and bond polarity determine the molecular polarity.

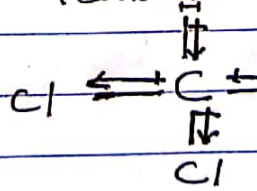
Molecular Polarity and Dipole Moment

Carbon tetrachloride (CCl_4)



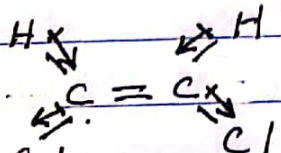
$\mu = 0\,D$

Trichloromethane $CHCl_3$ (Chloroform)



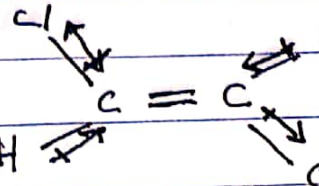
$\mu = 1.02\,D$

cis-Dichloroethene, $C_2H_2Cl_2$



$\mu = 1.90\,D$

Trans-Dichloroethene



$\mu = 0$

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Bond Angle

→ is the angle formed by two surrounding atoms with the central at the vertex.

Eg. Consider the water molecule, H_2O:



→ Ideal Bond Angles are observed when all the bonds around the central atom are identical and connected to the same type of atoms. If this is not the case, the bond angles deviate the ideal angles.

Total No. of valence electron Pairs	Bond Angle	Arrangement of electron pairs (e^- pair geometry)	No. of Bonding Pairs	No. of Lone Pairs	Molecular Formula	Shape of Molecule	Example
2	180°	Linear	2	0	AX_2	Linear	CO_2, $BeCl_2$, CS_2, HCN
3	120°	Trigonal Planar	3	0	AX_3	Trigonal Planar	BF_3, NO_3^- HCHO
3		>> >>	2	1	AX_2E	V-shaped (Bent or Angular)	SO_2, O_3, $SnBr_2$
4	109.5°	Tetrahedral	4	0	AX_4	Tetrahedral	CH_4, NH_4^+, SO_4^{2-}
4		>>	3	1	AX_3E	Triangular pyramid	NH_3
4		>>	2	2	AX_2E_2	V-shaped (Bent or Angular)	H_2O
5	90°, 120°	Trigonal Bipyramid	5	0	AX_5	Trigonal Bipyramid	PF_5, PCl_5
5		>> >>	4	1	AX_4E	Seesaw	SF_4, XeO_2F_2
5		>> >>	3	2	AX_3E_2	T-shaped	ClF_3
5		>> >>	2	3	AX_2E_3	Linear	I_3^-
6	90°	Octahedral	6	0	AX_6	Octahedral	SF_6
6		>>	5	1	AX_5E	Square Pyramid	BrF_5
6		>>	4	2	AX_4E_2	Square Planar	BrF_4^-, XeF_4

Exercise

1. Determine the molecular shape and ideal bond angles in:
   a) $COCl_2$ b) PCl_3 c) SF_2 d) CS e) H_2Se f) SbF_5 g) BrF_5
2. In which situations is/are the molecular shape and the electron set arrangement is/are same?
3. Arrange the following AF_n species in order of increasing F-A-F bond angles. BF_3, BeF_2, CF_4, NF_3, OF_2.
4. For molecules of general formula AX_n (where $n>2$) how do you determine if a molecule is polar?

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5. Predict the geometry of and bond angles (relative to the ideal angles) in the following molecules and ions.

a) ClO_3^+ b) ClO_2^+ c) ICl_2^- d) SOF_4 e) ClF_3

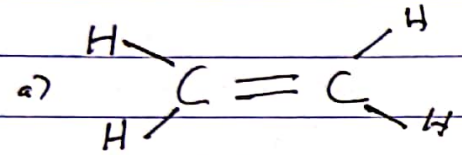
6. Draw molecular shapes for the molecules/ions in the above question.

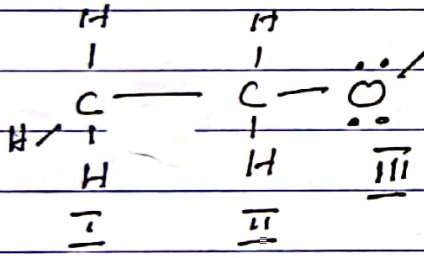
Note the following: The molecular shape of molecules with more than one central atoms are different in different parts of the molecule. For these type of molecules, it is easiest to find the molecular shape around one central atom at a time.

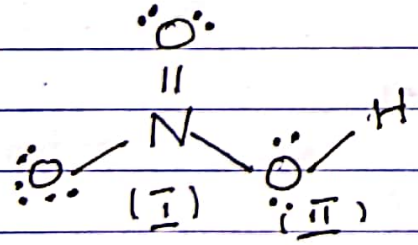
Eg. Consider a) Ethene

b) Ethanol

c) HNO_3

a)  → around each central atom the shape is trigonal planar.

b)  → three central atoms: I, II and III. I and II are tetrahedral. III is V-shaped or bent.

c)  → Two central atoms (I) and (II). At (I) is trigonal planar. At (II) V-shaped

Intermolecular Forces in Covalent Substances (Compounds and Elements)

There are two types attractive forces (electrostatic forces). They are: (i) Intramolecular forces (ii) Intermolecular forces

Intramolecular Force - is chem. bond (Ionic, covalent or metallic) is a force that exists within a particle (molecule or polyatomic ion) and affects the chem. properties of the species.

Intermolecular Forces - weak attraction forces. They exist bln the particles in substances. They influence physical properties of substances. They arise b/c of the attraction b/n molecules and atoms. The most important ones are:

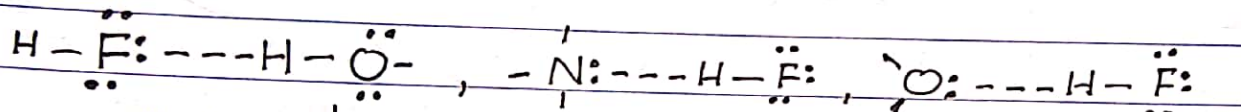
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(i) Dipole – Dipole Forces – IMAF that exist b/n permanently polar molecules. Their strength varies from 5 to 25 $KJmol^{-1}$.

Eg In b/n HCl molecules in liquid and solid form

$^{\delta+}H - Cl^{\delta-}$

(ii) Hydrogen Bonding – strength varies from 10 to 40 $KJmol^{-1}$. special type of dipole – dipole forces. Exist b/n molecules that have H atoms bonded (bound) to smaller sized, most electronegative atoms (F, O and N). The partially positive ($\delta+$) H of one molecule is attracted to the partially negative ($\delta-$) lone pair on the F, O or N of same or another molecule.

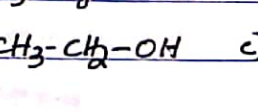


The broken lines represent H-bonds

(iii) Dispersion or London Forces

Intermolecular forces in which non-polar atoms or molecules interact by inducing dipoles in each other is known as London or dispersion forces. These classes of IMAF cause substances like [CO_2, Cl_2, noble gases, etc to condense and solidify. Their strength ranges from (0.05–40) $KJmol^{-1}$. Strength is dependent on surface area of molecules. Large surface area means stronger dispersion forces.

Exercise 3.11.

1. In which of the following substances do hydrogen bonds occur? Explain with the help of diagrams. A) CH_4 B) CH_3-CH_2-OH C) 

2. Identify the dominant IMAF that is present in each of the following substances and select the substances with the higher boiling point in each pair:

A) CH_3OH or CH_3CH_2OH

B) Hexane or cyclohexane

C) $MgCl_2$ or PCl_3

D) CH_3NH_2 or CH_3F

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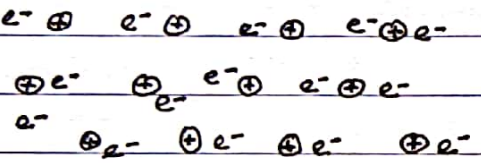
3. Which of the following type of is dominant in the following substances ?

A) ICl B) H_2O C) F_2 D) HBr

4. Compare and contrast IMAF with that of intramolecular bonding

Metallic Bonding

→ occurs in metals. It is the attraction b/n +vely charged core (Kernels) of metals and delocalized (conduction) electrons. It can be imagined as sea of electrons in which +vely charged metal ions are embedded.



Unlike ionic bonding, the metal ions are not held in place as rigidly as in ionic solids. Unlike covalent bonding, no particular pair of metal atoms is bonded through any localized pair of electrons. Rather, the valence electrons are shared among all the atoms in the substance which is held together by the mutual attraction of the metal cations for the mobile, highly delocalized electrons. In metals the bonding e^- are free to move throughout the three dimensional structure.

Properties of Metals

→ Malleable and ductile, Strong and durable, Good conductors of heat and electricity. Their strength is an indication that the atoms are difficult to separate; but malleability and ductility suggest that the atoms are relatively easy to move in various directions. Most metals are solids with high melting and boiling points.

Metallic bond: +ve ions in sea of electrons.

EXERCISE

1. Arrange K, Br_2, Mg and O_2 in increasing order of melting points. Explain why.
2. List four properties of a solid metal.
3. .

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