Molecular Structure
3 - Intermolecular Forces

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Purpose of Intermolecular Forces

Intermolecular force (IMF) is the force between molecules in any phase of matter. They help to determine physical properties of substances e.g. melting and boiling points (which helps to determine if the substance is solid, liquid or gas), surface tension, viscosity and solubility in different substances.

Intermolecular forces depend on the polarity of the molecule.

The three main physical properties that we will focus on will be:

- **Boiling and melting point**: More polar molecules will have a higher boiling and melting points.
- **Solubility**: Like dissolves like. Polar molecules will dissolve in polar substances.
- **Vaporization**: This is dependent on boiling point; the lower the boiling point the more the substance will vaporize. For this reason, most organic compounds are highly volatile (and can have odor).

Intermolecular Forces (IMF) and Bonding

Covalent and ionic substances have different kinds of intermolecular forces (IMF).

- Ionic Compounds: Due to the presence of cations and anions, all ionic substances have electrostatic forces or ionic forces. These are the strongest forces resulting in high melting points. We will not be discussing these more as it is understood that ionic forces are the strongest.
- Covalent compounds have three kinds of IMF forces (from lowest to highest strength):
  A. Dispersion forces
  B. Dipole-dipole forces
  C. Hydrogen bonding

  These forces depend on the polarity of the covalent bond. The higher the polarity the higher the IMF.

A) Dispersion Forces/Van der Waals Forces/ London Forces

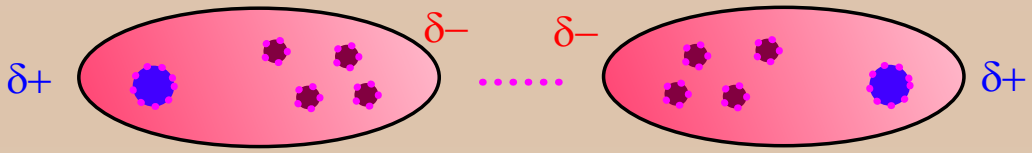
Dispersion force or any of the names listed above, is the IMF due to internal electron distribution in molecules. This is also called induced dipole.

This force occurs in molecules with high electron density, which could be because of a large atomic size or a molecule that has many atoms.

Atomic size: Consider the halogens: F_2, Cl_2, Br_2 and I_2. As one goes down the group the atomic size increases. The physical state of the element changes from gas to liquid to solid from F_2 to I_2. This is because the atomic size of iodine is so large that an internal charge distribution occurs. Because of this charge separation molecules interact differently.

The diagram below shows how the charge distribution occurs.

(*See next slide for physical properties*).



A) Dispersion Forces – Physical Properties

Below are the physical properties of halogens. It can be seen that as the molecular weight increases the boiling point increases thus resulting in fluorine as a gas and iodine as a solid.

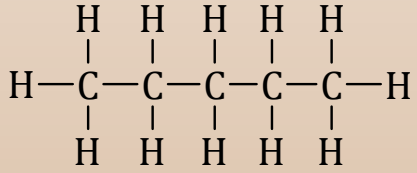
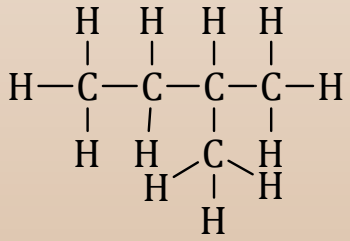
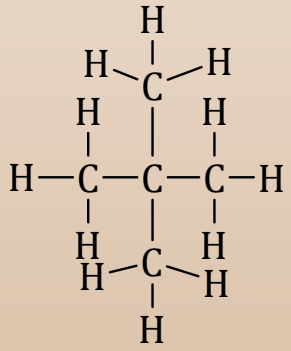
Molecule	Molar mass g/mol	Boiling point	State at Room Temp
F_2	38.0	-188	Gas
Cl_2	70.9	-34	Gas
Br_2	159.8	59	Liquid
I_2	253.8	184	Solid

A molecule can be multiatomic to have dispersion forces. For example, when comparing CH_4 (methane) and CH_3CH_3 (ethane) for boiling points, the second molecule, ethane, has more carbon atoms thus will exhibit higher dispersion forces and will have a higher boiling point. -358 ^oC for methane and -128 ^oC for ethane.

A) Dispersion Forces in Straight Chain vs Compact Molecules

For a compound with the formula, C_5H_{12}, we can draw three different structures, however, in each compound, the carbon atoms are bonded in a different structure. This changes the boiling point of the molecule.

The straight-chain compound has the strongest intermolecular forces and the highest heat of vaporization because it is most flexible and, therefore, most polarizable. Another way to look is that the straight chain compound has more surface area and thus more interaction for IMF.

		
<u>Pentane (straight chain 5 carbon structure)</u> Boiling point: 36 °C ΔH_{vap}: 25.8 kJ/mol	<u>Branched 5 Carbon</u> Boiling point: 28 °C ΔH_{vap}: 24.7 kJ/mol	<u>More branched 5 carbon structure</u> Boiling point: 9.5 °C ΔH_{vap}: 22.8 kJ/mol

B) Dipole Moment

Dipole moment **(μ)** is when a molecule can move in presence of an electric current. The higher the polarity of the molecule the higher the dipole moment. The polarity is a result of two factors: the difference in electronegativity of the atoms and the asymmetric shape of the molecule.

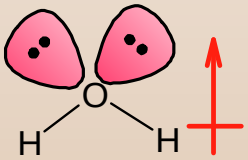
- Ionic compounds are inherently polar because of the presence of ions.
- Diatomic molecules of the same atom (H_2, Cl_2, I_2) are nonpolar as there is no difference is electronegativity.
- Any molecule that has polar covalent bonds can have dipole moment depending on its shape.
- E.g. HCl has stronger IM forces than HBr because the bond between HCl is more polar. H_2O is polar and CO_2 is nonpolar because of their respective shapes, bent vs linear even though they have polar bonds.

Formula	μ	Formula	μ
H_2	0	CH_4	0
Cl_2	0	CH_3Cl	1.87
HF	1.91	CH_2Cl_2	1.55
HCl	1.08	$CHCl_3$	1.02
HI	0.42	CCl_4	0
BF_3	0	NH_3	1.47
CO_2	0	H_2O	1.85

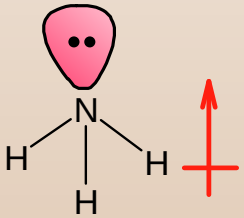
B) Determining Dipole Moment

Use the steps below to figure out dipole moment.

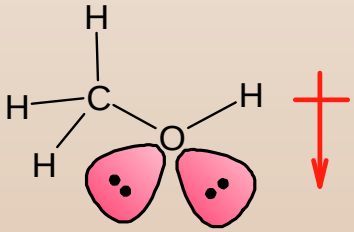
1. Write the Lewis structure
2. Determine the shape of the molecule
3. Identify the polar covalent bonds in the molecule
4. See if there is asymmetric pull in the molecule.



μ = 1.85 D

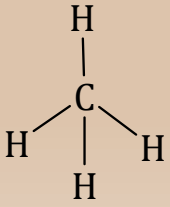


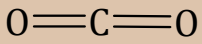
μ = 1.47 D

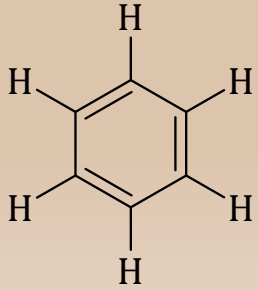


μ = 1.70 D

Symmetrical molecules don't have any dipole moment even though they may have polar bonds, for example CO_2.







B) Dipole Moment and Structure

The higher the dipole moment the stronger the dipole-dipole interaction between molecules.

The table below shows some molecules of the same molecular weight but different dipole moment and how that affects the boiling point of the substances.

(*Draw the Lewis structures of the molecules to see what shapes the molecules will be to help you with the dipole moment*).

Dipole Moments and Boiling Points			
Compound	**Formula**	**Dipole Moment**	**Boiling Point (°C)**
Propane	$CH_3CH_2CH_3$	0.1	-42
Dimethyl ether	CH_3OCH_3	1.3	-25
Chloromethane	CH_3Cl	1.9	-24
Acetaldehyde	CH_3CHO	2.7	21
Acetonitrile	CH_3CN	2.9	82

C) Hydrogen Bonding

Hydrogen bonding is a strong attractive force that exists between hydrogen atoms bonded to a very electronegative atom F, O, or N. In the representation below Y is F or N or N.

—Y—H ···· **Y**—

This is the strongest of all the IM forces. It holds the proteins and DNA together. Because of this force water is a liquid and has a high boiling point.

Comparison of IM Forces

The strength of IMF is from highest to lowest is as below:

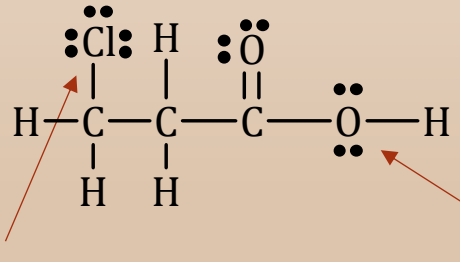
H-bonding > dipole-dipole> dispersion

In organic chemistry all these forces are key to understanding the physical properties of substances.

Solved Problem: Determining IM forces

What are the two key IM forces in the following molecule?

Answer



Dipole-dipole and hydrogen bonding

Solved Problem: Determining IM forces

What are the IM forces between the molecules given in the table?

Molecule	Answer
$CHCl_3$	Dispersion force dipole dipole forces
Br_2	Dispersion force
Ca_2NO_3	Electrostatic force
CH_3OH	Hydrogen bonding

Solved Problem: Determining IM forces

Which of the following has the highest dispersion force?

a) C_4H_{10} b) C_5H_{12} c) C_6H_{14} d) C_7H_{16} e) C_8H_{18}

Answer: The larger the molecule the higher the C_8H_{18}

Solved Problem: Determining Boiling point

Arrange the following molecules in increasing order of boiling point: $CHCl_3$, Br_2, Ca_2NO_3, and CH_3OH.

Answer: Strongest IMF is ionic thus Ca_2NO_3, followed by H-bonding, CH_3OH, dipole moment will be the next, $CHCl_3$, and finally the London forces is Br_2.
$Ca_2NO_3 > CH_3OH > CHCl_3 > Br_2$

Solved Problem: Determining Solubility

Which of the following molecules will be more soluble in water and which in hexane (C_6H_{14})?

a) C_4H_{10} b) CH_3OH c) Ca_2NO_3

Answer: Like dissolves like. Identify the IMF in molecules and determine solubility. H_2O has H-bonding while hexane has London forces. Among the three molecules: a) has London forces, b) has H-bonding and c) has ionic forces. a) will be soluble in hexane while b) and c) will be soluble in water.

Key Words/Concepts

- Electrostatic Force
- Dispersion force
- Dipole-dipole force
- Hydrogen bonding
- Effect of intermolecular forces on melting and boiling points and solubility of substances.