Polarity, Intermolecular Forces and Solubility of Molecules

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Special thanks to Ms Williams and Ms Matrella for their constant support and inspiration

Please note that these guides are a collation of my personal notes, teachers' notes, chemistry books, and websites such as chemguide, chemsheets, chemwiki and wikipedia.

Determining Polarity in Molecules

To determine whether a molecule is polar or not, we need to look at 2 main factors:

- Bonds involved within it
- Shape

Bonds

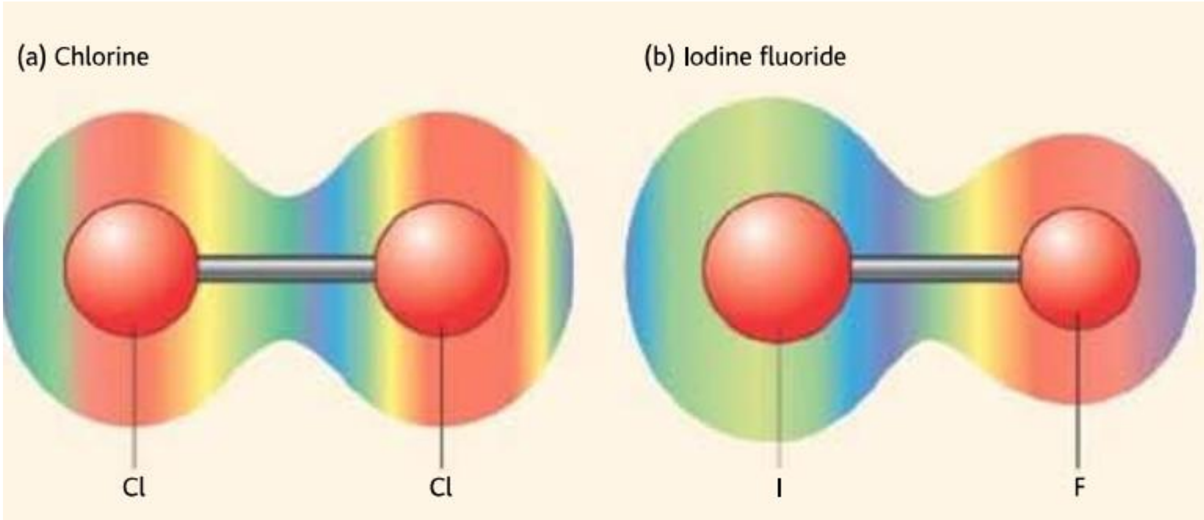
A key component in determining the polarity of a molecule is the polarity of its intramolecular bonds. To do so we need to look at the atoms involved in each bond and the electronegativity difference between them.

Electronegativity is a measure of the tendency of an atom to attract a bonding pair of electrons. The Pauling scale is the most commonly used. Fluorine (the most electronegative element) is assigned a value of 4.0, and values range down to caesium and francium which are the least electronegative at 0.7.

Electronegativity increases across a period because the number of charges on the nucleus increases. That attracts the bonding pair of electrons more strongly. As you go down a group, electronegativity decreases because the bonding pair of electrons is increasingly distant from the attraction of the nucleus.

H 2.1																
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8
Rb 0.8	Sr 1.0	Y	Zr	Nb	Mo 1.8	Tc	Ru	Rh	Pd	Ag 1.9	Cd 1.7	In	Sn 1.8	Sb 1.9	Te 2.1	I 2.5
Cs 0.7	Ba 0.9	La	Hf	Ta	W	Re	Os	Ir	Pt	Au 2.4	Hg 1.9	Tl	Pb 1.8	Bi 1.9	Po	At

If the difference between in the electronegativity of the atoms involved in a bond exceeds 0.5 it is said to be polar. This could be shown on a diagram. There is an equal distribution in Cl_2 since there is no difference in electrongeativty. But in IF, the red area around the F represents a stronger attraction between F and the shared electrons than I and the shared electrons. Hence the shared electrons are closer to Flourine.



The difference in electronegativity also determines the % of covalent and ionic character. The greater the difference, the greater the % of ionic character in the molecule.

Shape of the Molecule

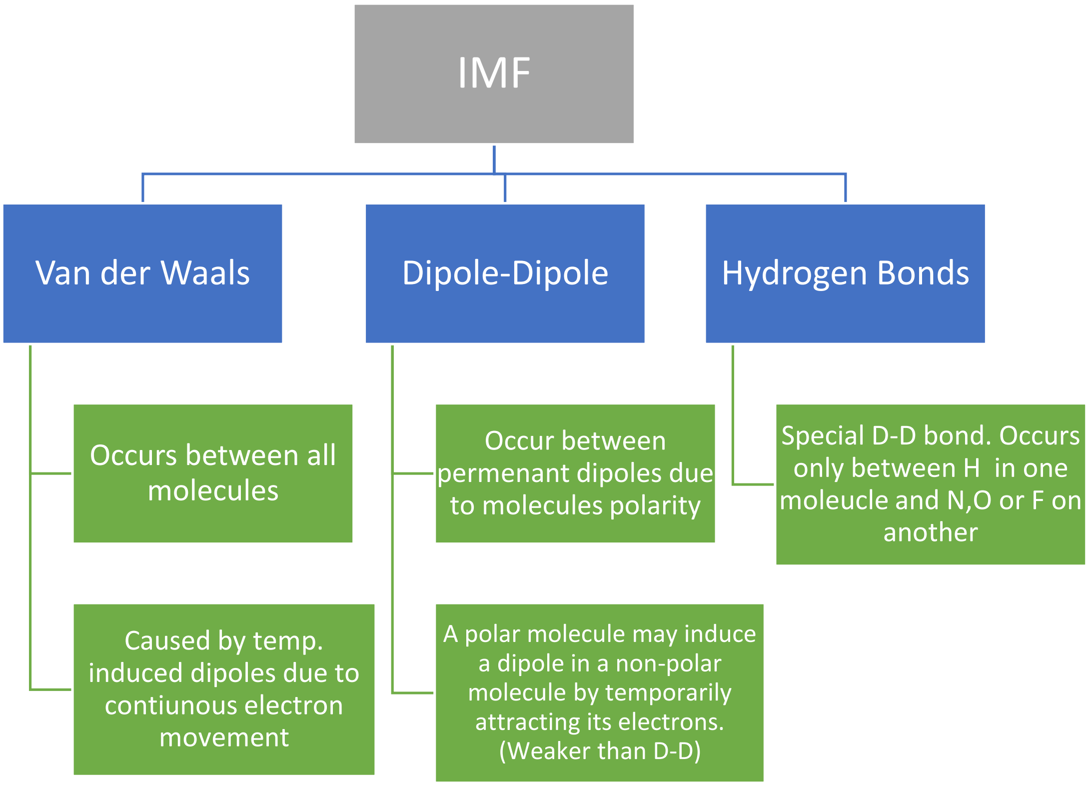
Previously we have discussed how to determine the shape of a molecule based on bonding and non-bonding pairs. Now we will use that to determine molecule polarity. As a rule, we can say that:

- If all the bonds in a molecule are non-polar, the molecule will not be polar
- If all the bonds in a molecule are the same type (e.g. C-H bond) yet its shape is symmetrical (i.e. no lone pairs/no distortion) the bond polarities are said to cancel out and the molecule is not polar
- If all the bonds in a molecule are the same type however its shape isn't symmetrical due to the presence of lone pairs/distortion, the bond polarities don't cancel out and the molecule is polar
- If all the bonds in a molecule aren't the same type, the molecule is probably polar

	Formula	Description	Example
Polar	AB	Linear molecules	CO
	HA	Molecules with a single H	HCl
	A_xOH	Molecules with an OH at one end	C_2H_5OH
	N_xA_y	Molecules with an N at one end	NH_3
Non-polar	A_2	All elements	O_2
	C_xA_y	Most carbon compounds	CO_2

Intermolecular Forces

Intermolecular forces (imf) are attractive forces between molecules. Intramolecular forces hold atoms together in a molecule (e.g. covalent bonds). Intermolecular forces are much weaker than intramolecular forces such as covalent bonds.



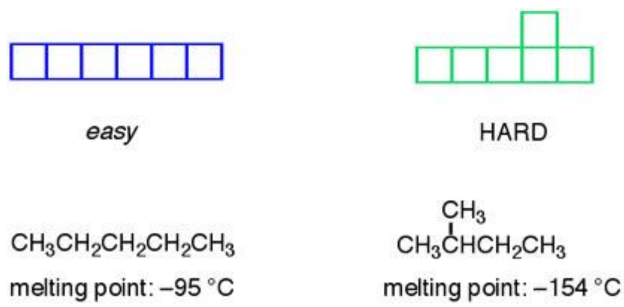
Van der Waals

In any atom or molecule the electrons are in continuous motion. As a result, at any instant the electron distribution may be slightly uneven. The momentary, uneven charge creates a δ+ in one part of the atom or molecule and a δ− in another. This temporary dipole can then induce a dipole in an adjacent atom or molecule. The two are held together for an instant by the weak attraction between the temporary dipoles. Stronger Van der Waals from:

- Higher surface area (e.g. large vs small electron cloud like branched and unbranched organic molecules with the same molecular structure)
- Having more electrons

Both of these factors will lead to a higher chance of δ- and δ+ forming.

Source: http://www.masterorganicchemistry.com/2010/07/09/chemical-tetris/



Dipole-Dipole

Polar molecules act as tiny dipoles because of their uneven charge distribution. A dipole is created by equal but opposite charges that are separated by a short distance. A polar molecule can induce a dipole in a non polar molecule by temporarily attracting its electrons. The result is a short-range intermolecular force that is somewhat weaker than the dipole-dipole force.

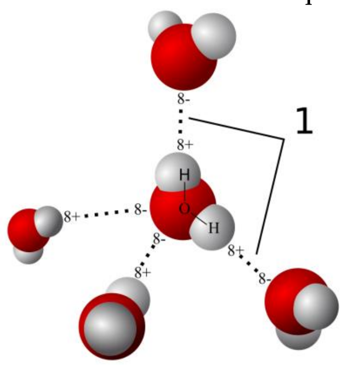
These can be made stronger by having a larger electronegativity difference between the atoms involved in the bond. E.g. HBr will have weaker dipoles than HCl.

Hydrogen Bonds

It forms between the hydrogen atom in a polar N-H, O-H or F-H bond and an electronegative O, N or F atom. Examples of molecules with H bonds are:

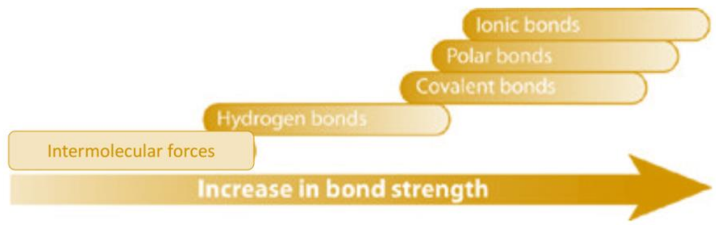
- NH_3 with 1 H bond per molecule as the N has only 1 lone pair available to bond
- HF with 1 H bond per molecule as there is only one Hydrogen to form H bonds
- H_2O with 2 H bonds per molecule as there is 2 lone pairs and 2 Hydrogens

The hydrogen bonds that form between water molecules account for some of the unique properties of water. The attraction created by hydrogen bonds keeps water liquid over a wider range of temperature than is found for any other molecule its size. Also as it has more H bonds per molecule than HF and NH_3 it has a higher boiling point than both of them. H bonds are also responsible for ice floating. As the temp. drops, the max number of H bonds are formed leading to a lot of space between the molecules compared to when the molecules have energy to move past each other (in liquid form). Hence ice is less dense than water. The '1' in the diagram represents the H bonds.



BOILING POINT & INTERMOLECULAR FORCES

As a liquid is heated, the kinetic energy of its particles increases. At the boiling point, the energy is sufficient to overcome the force of attraction between the liquid's particles. The particles pull away from each other and enter the gas phase. Boiling point is therefore a good measure of the force of attraction between particles of a liquid. The higher the boiling point, the stronger the forces between particles.



Solubility

- The solubility of a solute in a solvent is the number of grams of a solute that will dissolve in 100g of solvent at any given temperature to form a saturated solution.
- Solvent: A liquid that dissolves substances
- Solute: A substance that has completely dissolved
- Solution: Formed when a substance dissolves in a liquid
- Concentration: The mass of a solute that dissolves in 100g of solvent
- Miscible: When non-polar liquids mix completely
- Immiscible: 2 non-polar liquids form separate layers

When will a substance dissolve ?

A substance will dissolve if the intermolecular forces between the solute particles and the intermolecular forces between the solvent particles are overcome by the forces of attraction between solute-solvent particles.

Ionic Solute & Polar Solvent

When we have an ionic solvent such as water (ionic due to the polarity of the molecules) and an ionic solute such as NaCl (since it's an ionic compound) the slightly positive Hydrogens will be attracted to the chloride ions and the Oxygens will be attracted to the sodium ions. These attractions will cause the lattice to break down and the NaCl will hence dissolve. However NOT ALL the ionic solutes dissolve in water. Why? If we talk mathematically we can say:

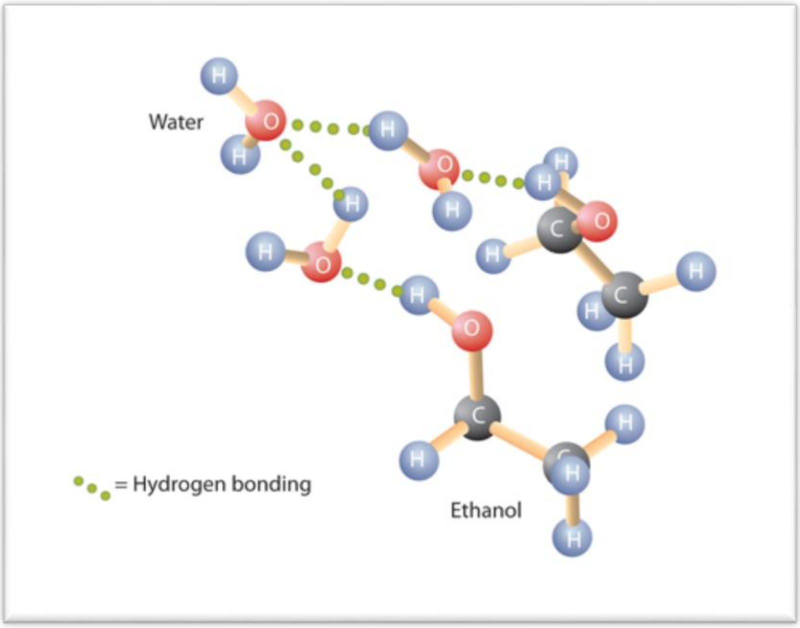
If . . .	Then . . .
Lattice energy = hydration energy	Substance dissolves, no temperature change
Lattice energy < hydration energy	Substance dissolves, solution gets warm/hot
Lattice energy > hydration energy	Substance dissolves, solution gets cold
Lattice energy >> hydration energy	Insufficient energy to break up lattice, substance is insoluble

Lattice Energy : energy required to break apart the giant ionic lattice

Hydration Energy : energy released when molecules arrange around an ion

Polar Solvent & Polar Solute

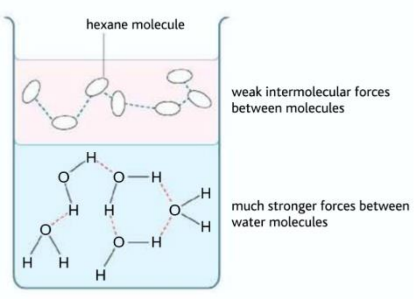
If we have water and a polar solute such as NH_3, H bonds will occur in this case between the Hydrogens, Nitrogens and Oxygens in the solution and the NH_3 will dissolve. The same concept applies with short chains of alcohols. However when the chain gets longer things change.



Solubility decreases with increasing chain length because of the non-polar part of the alcohol gets too big to dissolve in water. Hence a long chain alcohol such Hexanol would not dissolve in water.

Polar Solvent & Non Polar Solute

Water and Hexane aren't good friends. Hexane wouldn't dissolve in water because the strongest intermolecular forces in Hexane is Van der Waals while the strongest intermolecular forces in water is H bonds. Hence the hexane molecules cannot disrupt the strong hydrogen bonds between the water molecules.



The same concept applies with Iodine and other non polar solutes.

Non Polar Solvent & Non Polar Solute

I_2 and Hexane are soluble together. Both substances contain molecules held together by weak Van der Waals (London) forces. These weak forces form between molecules of both substances, and a mixture is easily formed.

Summary of Polarity

Solvent & Solute	Solubility
Polar & Polar	Great Combo (Unless long chain alcohol
Polar & Ionic	Soluble (Depending on Lattice Energy & Hydration Energy)
Polar & Non Polar	No
Non Polar & Non Polar	Great Combination