Intermolecular Forces

We have examined the bonding forces that hold atoms together, these are *intra*molecular forces. The forces are generally strong and to break them you perform a chemical reaction.

Force	Attraction	Energy / kJ mol^{-1}	Example
Ionic	Cation – Anion	400 - 4000	NaCl
Covalent	Nuclei sharing e-pair	150 - 1100	H-H
Metallic	Delocalised electrons	75 - 1000	Fe

There are also *inter*molecular non-bonding forces. These exist between one molecule and another and are generally weak (typically < 50 kJ mol^{-1}) and breaking those results in a physical change (i.e. solid → liquid → gas).

London Dispersion forces (van de Waal's forces)

- Instantaneous fluctuations in the electron density surrounding a molecule may induce a dipole in an adjacent molecule.
- The larger the surface area of the molecules the greater the dispersion forces.
- Typical energy 0.05 – 40 kJ mol^{-1}.
- Dispersion forces exist between all molecules.

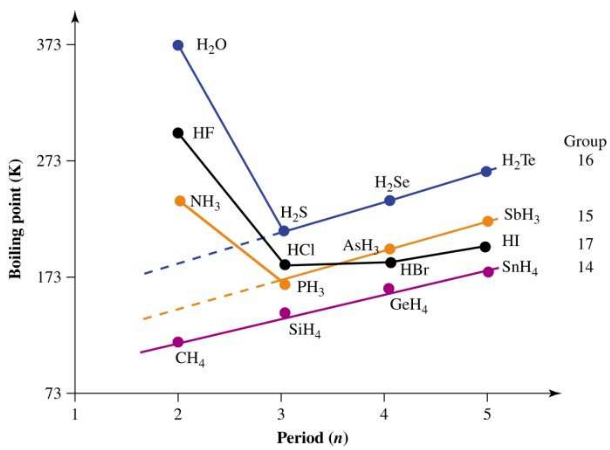
Dipole – dipole forces

- A covalent bond between atoms of different electronegativity will be polar. If a molecule containing polar bonds is asymmetric then the molecule will possess a permanent dipole.
- Dipoles of adjacent molecules align with one another resulting is an attractive force.
- Typical energy 5 – 25 kJ mol^{-1} (much less than a covalent bond).

Hydrogen Bonds

Hydrogen bonding arises from an unusually strong and directed dipole-dipole force. When H is bonded to a very electronegative element (F, O, N) the bond is polar covalent. H is unusual because with only one electron, it leaves a partially exposed nucleus (H has no other core electrons to shield the nucleus).

The bond can be thought of as forming between the hydrogen atom and the lone pairs of the F, N, or O in HF, NH_3 and H_2O, respectively.



Typical energy 10 – 40 kJ mol^{-1}.

F, O and N are all 2nd row elements, which convey certain properties:

- They are the most electronegative elements.
- They are small (only 2s, 2p in outer shell).
- They have lone pairs.

Water is perhaps the most unusual liquid. Each water molecule is H-bonded to **FOUR** other water molecules (donating 2 H-atoms and accepting two H-atoms to the lone pairs), forming a tetrahedral network (ice) and a loose tetrahedral network (liquid).

Force	Attraction	Energy / kJ mol^{-1}	Example
Dispersion forces	Fluctuations in e^- cloud	0.05 - 40	All molecules
Dipole-dipole	Partial charges	5 - 25	H-Cl
H-bonding	X::::H-X	10 - 40	H_2O

Question: Explain the trend in the table in terms of the type and size of intermolecular forces present.

Substance	ΔH_{vap} /kJ mol^{-1}	H-bonds?	M.W.
Butane, $CH_3CH_2CH_2CH_3$	**22**		
Diethyl ether, (C_2H_5)-O-(C_2H_5)	**27**		
Methanol, CH_3OH	**38**		
Ethanol, CH_3CH_2OH	**43**		
Water, H_2O	**44**		
Decane, $CH_3(CH_2)_8CH_3$	**51**		

Question: Which of the following substances show H-bonding? Draw the structure for those that do.

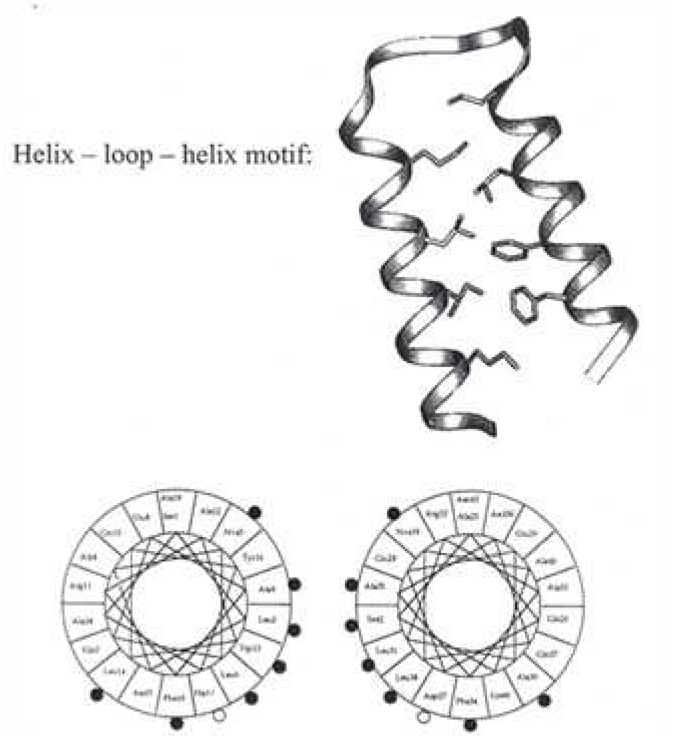
a) C_2H_6 b) CH_3OH c) CH_3CONH_2 d) H_2S e) HCl f) NH_3

Note: I will briefly discuss the material in the following box as an illustration of how we may use our knowledge of intermolecular forces to design molecules with particular characteristics. The information in the box is not examined in this part of the course.

Engineering a protein

Eg Ser-Leu-Aad-Ala-Nva-Leu-Gln-Glu-Ala-Phe-Arg-Ala-Trp-Leu-Gln-Tyr-His-Ala-Ala-Ala-Ala-Ala-Ala-Ala-Gln-Asp-Gln-Glu-Ala-Leu-Arg-Ala-Phe-Ala-Aad-Gln-Leu-Nva-Ala-Lys-Ile-Asn

- Ala-Ala-Ala-Ala – introduces a loop.
- One turn of helix ~ five amino acids.
- Hydrophobic cavity on inside.
- Salt bridge included His17-Asp27



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