

## COVALENT STRUCTURES: SHAPE & BOND ANGLE

### VSEPR theory

Electrons will arrange themselves around a central atom as far apart as possible (because they repel)

- May be in BONDED pair, NON-BONDED pair or MULTIPLE BOND

electron domains.

$2x$  or  $3x$  bond = ONE ELECTRON DOMAIN / CNC.

2 CNCs / Electron Domains

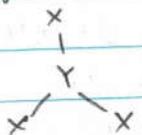
Linear



$180^\circ$

3 CNCs / EDs

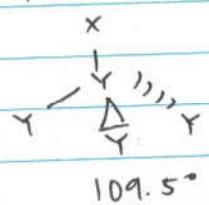
Trigonal planar



$120^\circ$

4 CNCs / EDs

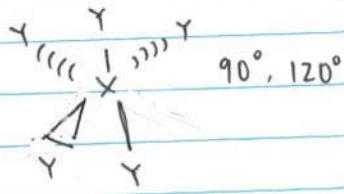
Tetrahedral



$109.5^\circ$

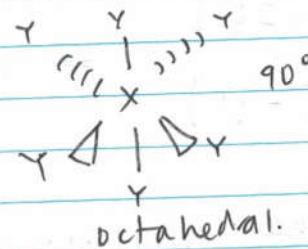
5 CNCs / EDs

Trigonal Bipyramidal



$90^\circ, 120^\circ$

6 CNCs / EDs



Octahedral.

non bonded pairs

also take up

space.

angle  $\downarrow 2.5$  for each non-bond pair.

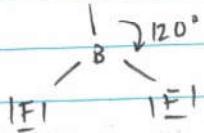
### Bond polarity & molecular polarity

molecular polarity is the result of individual bond polarity within a molecule AND the shape of the molecule itself

↳ some molecules may have polar bonds but are symmetrical = CANCEL.

$BF_3$

non-polar



Square planar (2 bpairs, 2 lone pairs)

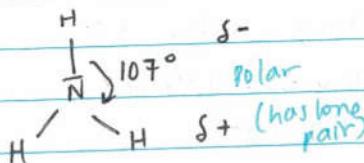
pyramidal (3 pairs + 1 unpaired)

non-linear / bent (2 pairs and 1 lone pair)

v-shaped ( $117.5^\circ$ )

square pyramidal (5 pairs, 1 unpaired)

$NH_3$

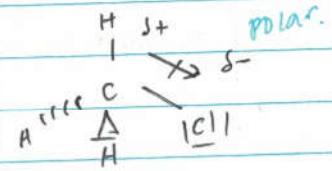


$s-$

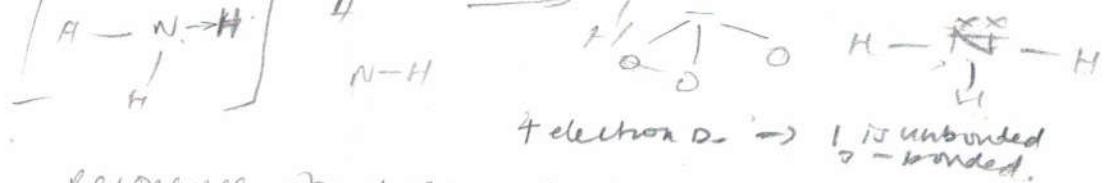
polar

$s+$  (has lone pair)

$CH_3Cl$



polar.



### RESONANCE STRUCTURES

Resonance structures,  $\text{N}_2\text{O}_4$

Carbon + silicon,

giant  
valent.

more possible position for a double bond in a molecule/ion

↳ individual structures are resonance forms

↳ actual structure is called resonance hybrid

### delocalisation of electrons

when there are a no. of p-orbitals (ie  $\pi$  bonds) on neighbouring atoms in a molecule/ion + a few resonance structures can be drawn.

$\pi$  cloud forms rather than  $\pi$  bond = electrons are delocalised!

THE SPREADING OF  $\pi$  ELECTRONS

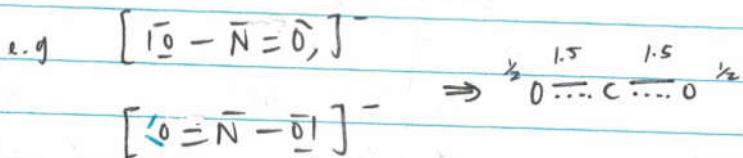
ACROSS 2+ ATOMS.



$\sigma$  bonds are 1.5 bonds

$\square$  bond length/strength is between single/double bond

$\square$  very stable structure!



### GIANT COVALENT STRUCTURES: ALLOTROPIES OF CARBON

diamond: 4 Bonds between carbon, = strength, all sigma

↳ tetrahedral structure

↳  $\text{sp}^3$  hybridized (4 electron domains)

↳  $\times e^-$  delocalized  $\therefore \times$  conductivity

↳ strong covalent bonds =  $\text{mpf} \propto \uparrow \uparrow$

covalently bonded  
Interlocking structure  
is very strong.

graphite: 3 Bonds between carbon (sigma) = layers

↳ hexagons that interlock

↳  $\text{sp}^2$  hybridized

↳ one  $e^-$  in p-orbital  $\rightarrow$  overlaps w/ other p-orbitals to form  $\pi$  cloud

↳ within layer = strong  
between = weak London forces

✓ Invariant layers  $\uparrow$  ✓ conducts  $\uparrow$ , 'p' electrons more

## GIANT COVALENT STRUCTURES: GRAPHENE

### graphene

- layer of planar carbon atoms in **HEXAGONAL** arrangement
- similar to graphite =  $sp^2$  hybridized
- giant covalent structure (crystalline lattice, 2D)
- ✓ conduct  $\downarrow$ , 'p' electrons delocalized
- ✓ strong ✓ flexible ✓ transparent

### $C_{60}$ / Bucky Balls

- spherical carbon molecules e.g. buckminsterfullerene (60 C atoms)
- 3 strong sigma bonds, arranged as pent/hex-agons  
↳ joint to make ball shape
- ↳  $sp^2$  hybridized
- ✓ strong ✓ light but **weak** van der waals hold molecules together  
mpf much lower than graphite/diamond.
- unbound 'p' electron - forms pi cloud - conduct  $\downarrow$  - not as good as layers.

### Silicon

- same as diamond BUT no allotropic behavior - only covalent bonding.

### $SiO_2$

- Si bonds to 4 O<sub>-</sub> atoms in tetrahedral structure
- O bonds to 2 Si atoms.
- covalent GIANT structures ✓ HIGH mpf X conduct  $\downarrow$

## SIGMA & PI BONDS

single covalent bonds are sigma ( $\sigma$ ) → an axial, head-on/end-on overlap of 2 atomic hybrid orbitals

→ electrons distributed symmetrically around a line  $X - X$

a double covalent bond is a  $\sigma$  AND a sideways overlap of 2 non-hybridized p-orbitals

this happens ABOVE + below the sigma bond ( $\pi$ , pi bond)

In a triple covalent bond →  $\sigma + 2\pi$

## HYBRIDISATION

is the combining of atomic orbitals to produce new hybrid bonding orbitals

↳ when atoms covalently bond, they share electrons, but this happens by overlapping orbitals.

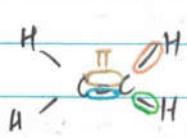
↳ BUT: some are in...

- ① different orbitals (s, p, d, f)
- ② different shapes.

so. Atoms create a NEW bonding orbital

a combination / HYBRID of types (s, p, d, f), energy and shape of orbital.

e.g. Ethene



$2p \begin{smallmatrix} 1 \\ | \\ 1 \end{smallmatrix} \quad 1 \quad 2p \begin{smallmatrix} 1 \\ | \\ 1 \end{smallmatrix} \quad 1 \quad 1$   
2s  $\begin{smallmatrix} 1 \\ | \\ 1 \end{smallmatrix}$                   2s  $\begin{smallmatrix} 1 \\ | \\ 1 \end{smallmatrix}$

GROUND

EXCITED

$\begin{smallmatrix} p & 1 \\ | & 1 \\ s & 1 \\ | & 1 \\ p & 1 \\ | & 1 \end{smallmatrix}$   
HYBRIDISED

tetrahedron

this leaves ONE unhybridised

trigonal

4 (NCS -  $sp^3$ ) 'p' electron to form a pi bond!!

planar

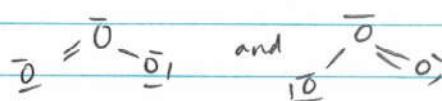
anything with 3 NCS -  $sp^2$

linear

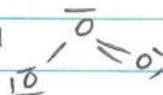
2 (NCS -  $sp$ )

lower energy level, more stable, harder to break

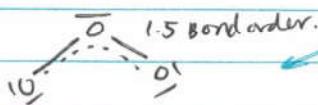
## OZONE ( $O_3$ )



and



make



bond strength =

bond has same energy

UV A - high wavelength, low frequency ∴ LOW ENERGY.] ozone stays B/1A

B

C - low wavelength

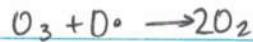
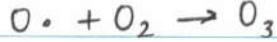
] oxygen stays C

formation

depletion



OVERALL  
 $O_3 + O^\cdot \rightarrow 2O_2$   
 depletion  
 catalysed



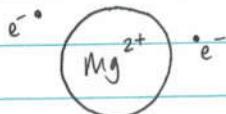
reaction with  $CCl_2F_2$

$NH_3$



## METALLIC BOND

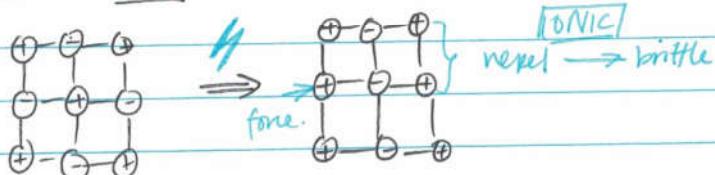
metals generally have low electronegativity (and like to be oxidized)



metallic bond = bond between positive metal ion and a sea of delocalized electrons.

BONDING IS MOBILE

↳ when you hit them.



but metals are MALLEABLE (make into shapes)

↳  $\text{e}^-$  constantly moving, keeping the bonds

what makes metal strong?

DUCTILE (pull into wires)



LARGER



SMALLER ionic radius

↳ HIGHER charge density:

but same charge: (same charge, but larger atom)  
( $2+$ ) →

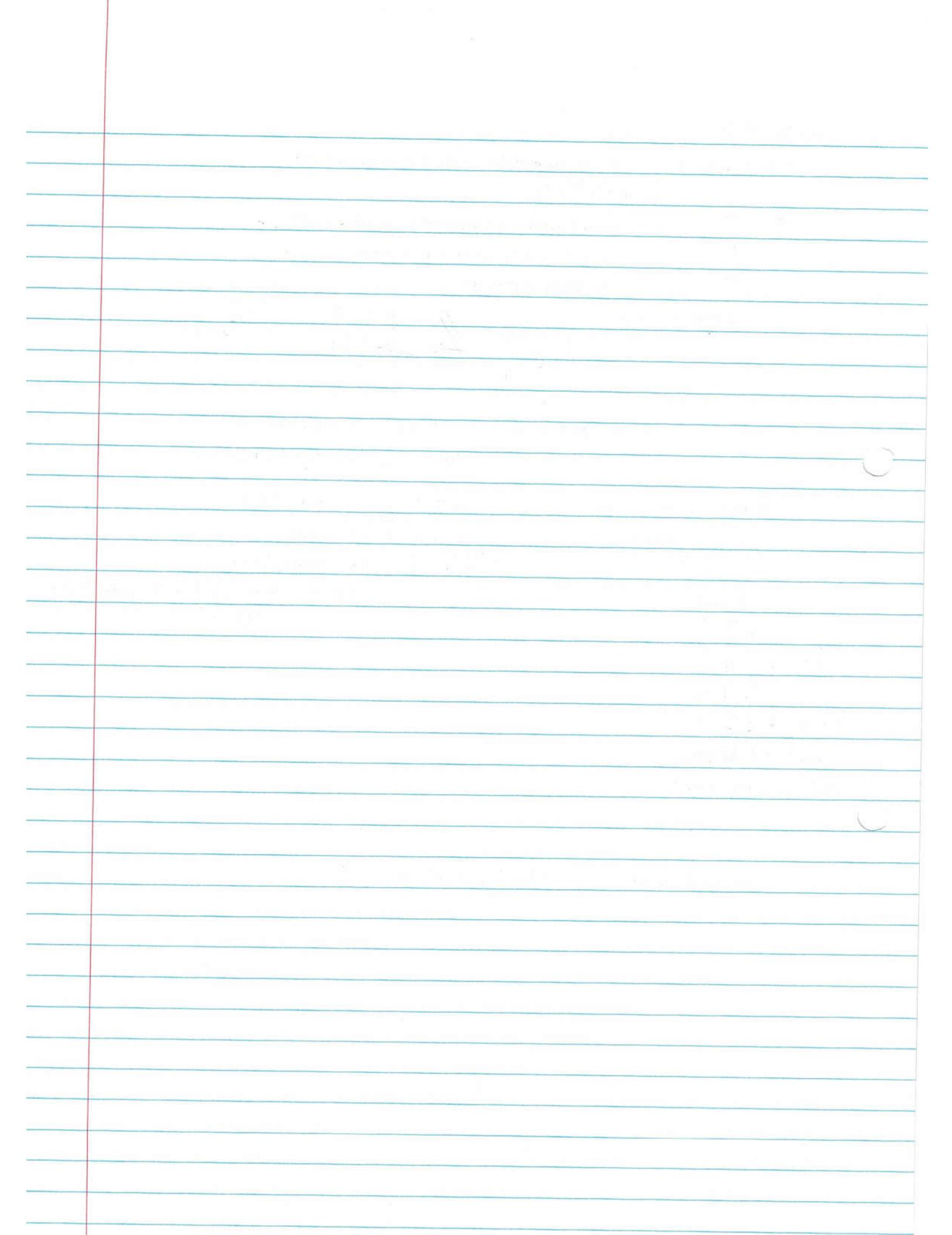
increase  
in ionic  
radius



DECREASE CHARGE DENSITY

LOWER MELTING POINT.

alloys are mixed metals or a metal with non-metallic element



## BONDING

### IONIC BONDING & STRUCTURE.

metals donate valence electrons, non-metals gain valence electrons = FULL OUTER SHELL.  
 ↳ +ve ions (cations)      ↳ -ve ions (anions)  
 ↳ held together by electrostatic forces.



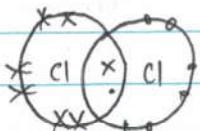
ions w/ more than 1 element = polyatomic.

$\text{HCO}_3^-$	$\text{SO}_4^{2-}$	$\text{PO}_4^{3-}$
$\text{ClO}_3^-$	$\text{NH}_4^+$	$\text{CN}^-$
$\text{OH}^-$	$\text{CO}_3^{2-}$	$\text{NO}_3^-$

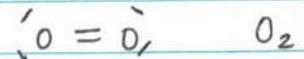
- an ionic bond is due to the electrostatic attraction between oppositely charged ions.
- they are usually solids with lattice structures, and have solid crystalline properties
  - ↳ have HIGH melting points due to strong electrostatic attraction.
- conduct electricity in aqueous/molten state - ions free to move
- dissolve in water due to polar nature
- electrolytes solvents (power source + industrial process)

### COVALENT BONDING

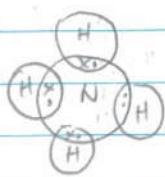
happens between a PAIR of electrons and positively charged nuclei held together by mutual attraction of the pair of electrons to the nuclei.



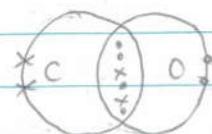
and may have multiple bonds



coordinate bonds are formed when ONE ATOM supplies BOTH shared electrons to form covalent bond. ( $\text{NH}_4^+$ ,  $\text{H}_3\text{O}^+$ ,  $\text{CO}$ )



bond length decreases  
bond strength increases



as the no. of shared electrons ↑↑

$$\frac{1}{\text{bond strength}} \propto \text{bond length}$$

### IONIC OR COVALENT?

electronegativity is the ability of an atom to attract an electron (covalent bond?)

large electronegativity = ionic. ( $\Delta > 1.8$ )

↳ closest to Fluorine = most electronegative.

↳ similar electronegativity = less polar.

greater  $\Delta$  in electronegativity = more polar (e.g. water)

## COVALENT STRUCTURES

electrons exist in pairs (xx, x<sup>-</sup>, -)

- most elements follow the octet rule (CONF. conference)

- others can have less than 8e (Be, B, Al, bernal)

- others expand make more than 8e (P, S, Cl)

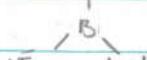
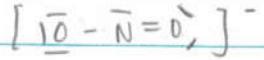
working out Lewis structures:

① total no. of valence electrons  $\div 2$  = pairs

② link the central atom + other atoms.

③ add more pairs round each atom (unless H, Be (4e), B & Al (6e))

④ add double bonds. ⑤ if P, S, Cl: add electrons to central atom.



But what if there's more than one Lewis structure? Ans: FORMAL CHARGE.



$\hookrightarrow$  FC = charge of atom if all molecule had = electronegativity.



FC = no. of valence e<sup>-</sup> - no of bonds - no. of bonding e<sup>-</sup>

$$\text{a. } \text{FC}([\text{N}]) = 5-2-4 = -1$$

$$\text{FC}(\text{N}) = 0$$

$$\text{FC}(\text{N}) = -2 \text{ too far from O.}$$

$$(\text{N}_1) = 5-4-0 = +1$$

$$(\text{N}_1) = +1$$

$$(\text{N}_1) = +1$$

$$(\text{O}) = 6-2-4=0$$

$$(\text{O}) = -1$$

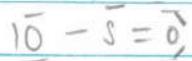
$$(\text{O}) = +1$$

lower FC = most stable structure (less charge transfer)

A + B have same lowest FC, so you must choose the one where

the negative values of FC is on the MOST electronegative atom

O is the most electronegative. B is preferred.



$$\text{FC}(\text{O}) = 6-1-6 (-1)$$

$$\text{FC}(\text{O}) = 6-2-4 -0$$

$$(\text{S}) = 6-3-2 (2+)$$

$$(\text{S}) = 6-4+2 \approx 0$$

$$(\text{O}_1) = 6-2-4 = 0$$

$$(\text{O}) = 6-2-4 = 0$$

## INTERMOLECULAR FORCES

forces between covalent molecules.  
ALL = VANDER WAALS FORCE

{ London forces  
dipole-dipole  
H+ bonds.

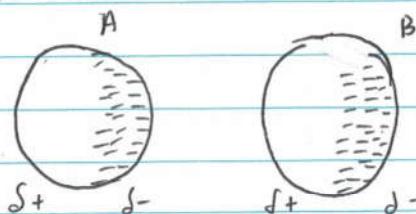
simple molecular compounds

STRONG INTRAMOLECULAR forces (within molecule)

WEAK INTERmolecular forces

STRONG COVALENT bonds BETWEEN ATOMS.

### LONDON FORCES

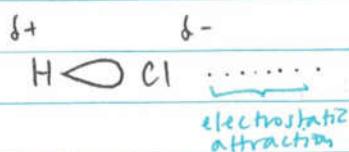


movement of electrons creates a temporary dipole which induces a dipole in a neighbouring molecule.  
Temporary induced dipole.

STRENGTH = more electrons ( $\propto$  Mr)

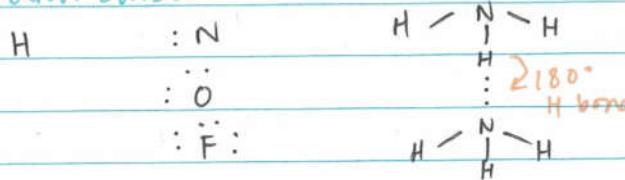
= surface area of contact  $\approx$   $\uparrow$  CONTACT  $\uparrow$  STRENGTH  $\uparrow$  mp.  
(ability to get closer)

### DIPOLE-DIPOLE



formed due to a permanently induced dipole (the molecules are polar)  
STRENGTH: depends on difference in electronegativity (how polar)

### HYDROGEN BONDS



it is an interaction between a hydrogen atom and a lone pair of N, O or F.  
STRENGTH: no. of H bonds

### property of hydrogen bonds

- HIGH B.P.
- HIGH surface tension (adhesive)
- SOLID less dense than liquid.

no of lone pairs.

open lattice = every H can bond w/ another atom.

