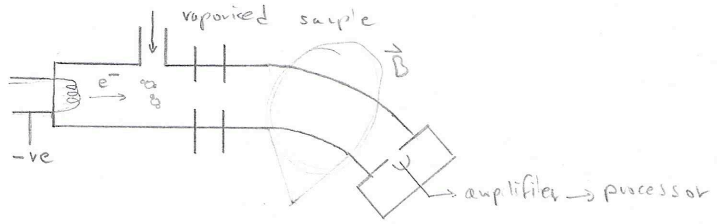
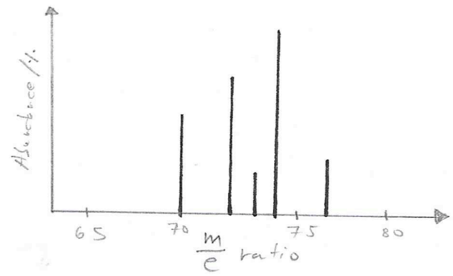
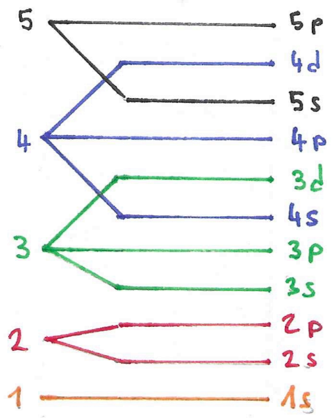
- formulas : isotopic → atomic → empirical → molecular

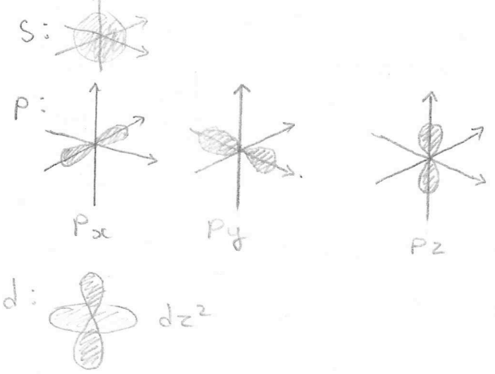




- molecules can fragment
- also Z^{+2} and more but those have much ↓ $\frac{m}{e}$, for Z^{+1} $M_i = \frac{m}{e}$

- ΔHi influenced by
  - ↳ size of Q on nucleus
  - ↳ distance of outer e^- to nucleus
  - ↳ shielding effect of inner e^-



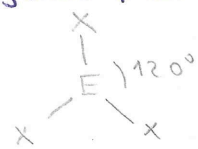


- Metalic bonding influenced by
  - ↳ +Q on ions ↑
  - ↳ size of metal ions ↓
  - ↳ no of delocalised e^- per atom ↑

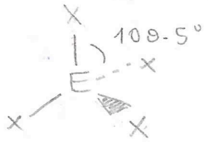
- Aufbau principle - orbitals fill low E to high E
- Pauli exclusion principle - 2 e^- in one orbital must have opposite spin

2 e^- regions linear

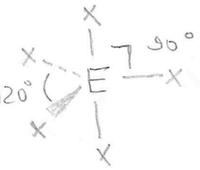
3 e^- regions trigonal planar



4 e^- regions tetrahedral



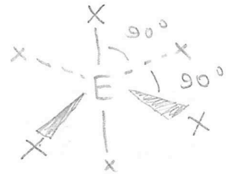
5 e^- regions trigonal bi-pyramidal



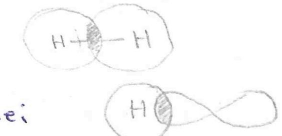
- e^- repulsion:

lone pair - lone pair > lone pair - bond pair > bond pair - bond pair

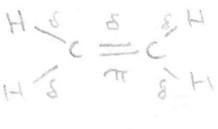
6 e^- regions octahedral



- covalent bonds
  - ↳ σ - sigma - head on interaction
    - equidistant between nuclei

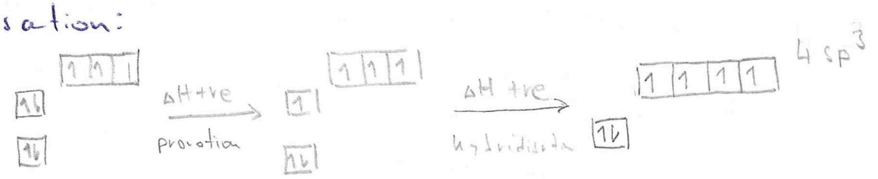


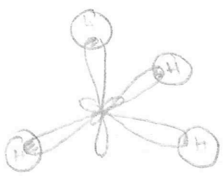
  - ↳ π - side on interaction
    - avg e^- density further from nucleus ∴ weaker



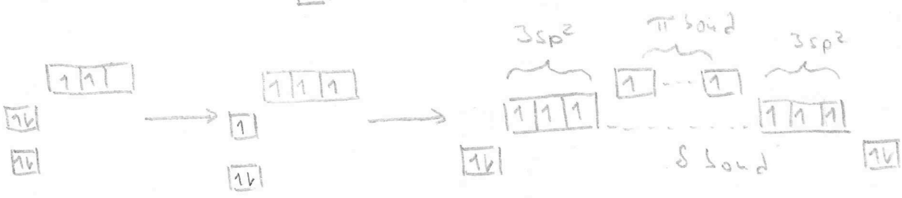
- hybridisation:

CH_4





C_2H_4

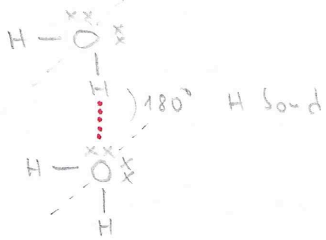


- intramolecular – covalent, dative, ionic, metallic
- intermolecular – H bonds, permanent dipole interactions
  - london dispersion forces
- electronegativity – measured on pauling scale
- to be polar: must have polar bonds (ΔX), and non symetrical

eg.) NH_3

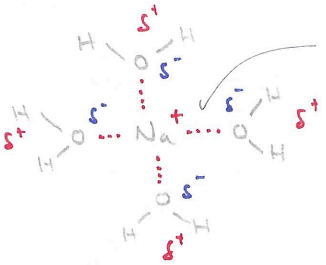
- dispersion forces: – e^- position fluctuate ∴ give rise to instantaneous dipole
  - instantaneous dipole induces dipole in surrounding molecules
  - dipoles now interact and establish weak bond
- H bond – H bonded to strong X atom: F, O, N
  - ↳ HF – strongest H bond, biggest ΔX
    - limited by no of H to 1. bond
  - ↳ H_2O – can form 2 H bonds of medium strength
  - ↳ NH_3 – weakest H bond
    - limited by no of e^- pairs to 1 bond

H bond allways at 180°



- in solution (not a complex)

$NaCl_{(s)} \xrightarrow{aq} NaCl_{(aq)}$



ionic – permanent dipole interaction stronger then H bond gives –ve ΔH_{hyd}

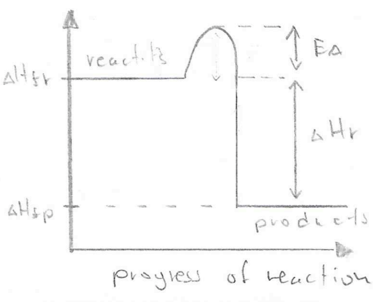
- polar molecules attract reactants ∴ ↑ reactive
- ideal gas – no forces of intermolecular attraction
  - atoms are ∞ small in ∞ vol
  - all collisions are perfectly elastic

} high temp, low pressure

- Boyles law: $PV = k$ @ const. T + n
- Charles law: $\frac{V}{T} = k$ @ constant P + n

T – allways in kelvin!
0k = –273°C

- general gas equation $PV = nRT$ R – universal gas constant
- vapor pressure P_{vapor} – if $P_{vapor} = P_{atm}$ then boiling occours
- molecule not polar if – vector sum of potentials = 0 ∴ symetrical
- E profile diagrams



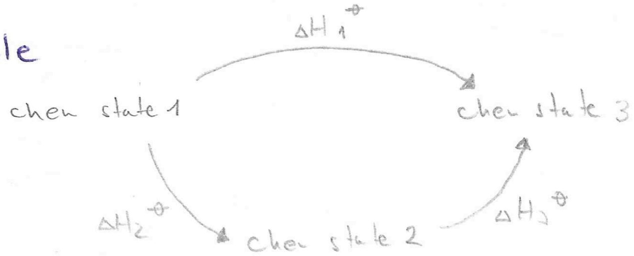
$Q = -mc\Delta T$

$\Delta H = \frac{Q}{n}$

ΔT +ve ΔH –ve

ΔT –ve ΔH +ve

- Hess cycle



$\Delta H_1 = \Delta H_2 + \Delta H_3$ provided initial + final conditions are same

- $\Delta H_r^{\ominus}$ - standard enthalpy change of reaction
  ↳ enthalpy change when formula amount of reactants react to give products under standard conditions. reactants + products in standard state
- $\Delta H_f^{\ominus}$ - standard enthalpy change of formation
  ↳ 1 mol of compound/substance is formed from its elements in their standard state under standard conditions
- $\Delta H_c^{\ominus}$ - standard enthalpy change of combustion
  ↳ 1 mol of substance is burnt in excess O_2 under standard conditions reactants + products in standard state
- $\Delta H_n^{\ominus}$ - standard enthalpy change of neutralisation
  ↳ strong monoprotic acid : $H^+_{(aq)} + OH^-_{(aq)} \longrightarrow H_2O_{(l)}$ $\approx -57\,kJ\,mol^{-1}$
  ↳ 1 mol of H_2O is formed by reaction of acid with alkali under standard conditions
- $\Delta H_{at}^{\ominus}$ - standard enthalpy change of atomisation
  ↳ 1 mol of gaseous atoms is formed from its elements in their standard state under standard conditions
- $\Delta H_{sol}^{\ominus}$ - standard enthalpy change of solution
  ↳ 1 mol of ionic solid dissolves in sufficient H_2O to give ∞ dil solution
- $\Delta H_{hyd}^{\ominus}$ - ~~Standard~~ enthalpy change of hydration
  ↳ 1 mol of specified gaseous ion dissolves in sufficient H_2O to give ∞ dilute solution (account 1 for each ion)
- $\overline{BE}$ - energy required to brake 1 mol of specific bonds (only in gaseous!)
- ΔH_{i1} - first ionisation energy
  ↳ E needed to remove $1e^-$ from each atom in 1 mol of gaseous atoms to form 1 mol of gaseous 1+ ions

- reduction - loss of O_2 - gain of e^- - ↓ ON   reducing agent - oxidised itself
- oxidation - gain of O_2 - loss of e^- - ↑ ON   oxidising agent - reduced itself
  ↳ 1.) ON of element = 0
  ↳ 2.) Σ ON of species = Q
  ↳ 3.) group 1 = +1   group 2 = +2
  ↳ 4.) ON of H = +1 except metal hydrides
  ↳ 5.) ON of O = −2 except F_2O and peroxides O_2^{2-}
  ↳ 6.) ON of F = −1
  ↳ more χ (electro −ve) takes the −ve ON

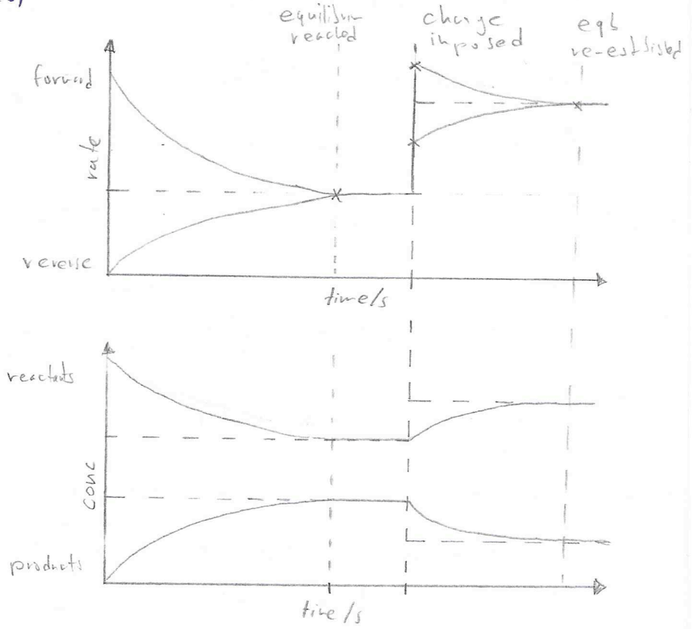
- dynamic equilibrium – $V_{forward} = V_{reverse}$
  - net conc of products + reactants is constant
  - temp + pressure are constant
  - reaction is in a closed system

- equilibrium constant – k_c $\qquad mA + nB \rightleftharpoons pC + qD$
  ↳ only affected by temp!
  ↳ invariant with conc of reactants/products $\qquad k_c = \dfrac{[C]^p[D]^q}{[A]^m[B]^n}$
  ↳ solids not included!

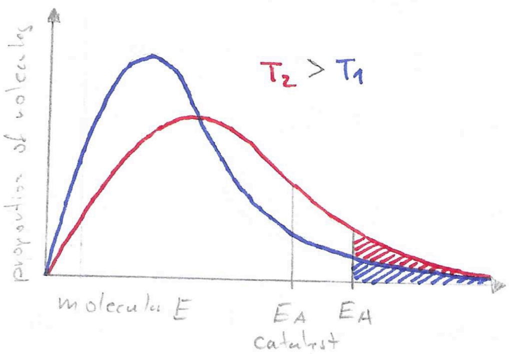
- mole fraction – mf $\qquad mf_A = \dfrac{n_A}{n_{total}} \qquad pp_A = mf_A \times P_{total}$
- partial pressure – pp
- equilibrium constant – k_p $\qquad k_p = \dfrac{(pp\,C)^p(pp\,D)^q}{(pp\,A)^m(pp\,B)^n}$
  ↳ also only dependant on temp

- Haber process: $N_{2(g)} + 3H_{2(g)} \rightleftharpoons 2NH_{3(g)}$ $\quad \Delta H_r = -92\ kJ\ mol^{-1}$
  ↳ iron catalyst at 200 atm 400 °C

- Contact process: $2SO_{2(g)} + O_2 \rightleftharpoons 2SO_{3(g)}$ $\quad \Delta H_r = -197\ kJ\ mol^{-1}$
  ↳ V_2O_5 catalyst 1-2 atm 400-500 °C



- factors affecting rate:
  ↳ concentration of reactants
  ↳ pressure
  ↳ temperature
  ↳ catalyst



increase of 10°C (K) roughly doubles the rate

- catalysis
  ↳ homogenous – catalyst + reactant in the same state
    - usually redox reaction – catalyst regenerated
    - $S_2O_8^{2-} + 2I^- \longrightarrow 2SO_4^{2-} + I_2$ catalyst Fe^{2+}/Fe^{3+}

  ↳ heterogenous – catalyst + reactant in different state
    - contact process, haber process, H_2O_2 decomposition
    - $2H_2O_{2(aq)} \xrightarrow{MnO_{2(s)}} 2H_2O_{(l)} + O_{2(g)}$
    - reaction occours only on surface of catalyst
    - adsorbtion, bonds weaken, desorption

- enzyme - biological catalyst
  - ↳ more efficient than inorganic catalist + doesnt produce bi-product
  - ↳ highly specific + only works in mild conditions 35°C 7pH atm pressure

urease $(NH_2)_2CO + H_2O \longrightarrow 2NH_3 + CO_2$

- alkali - base dissolved in H_2O
- Brøwnsted-Lowry: acid - H^+ donor
  base - H^+ acceptor
- strong acid/base dissociates almost compeletly
- weak acid/base dissociates only partially

$$\underset{\text{base}}{NH_{3(aq)}} + \underset{\text{acid}}{H_2O_{(l)}} \rightleftharpoons \underset{\text{acid}}{NH_{4(aq)}^{+}} + \underset{\text{base}}{OH^{-}_{(aq)}}$$

conjugate pairs (acid - base)