

COURSE : CHEM 202 - SUMMER 2010

FINAL GRADE : 87

NOTE: This is not a 'complete' summary. I've only written what I judged important, with some tips...

To do well you have to practice your knowledge in problems

Done by ERIK VZ (you can add me on facebook, if you have questions...)

Please visit the following blog www.blueaub.blogspot.com

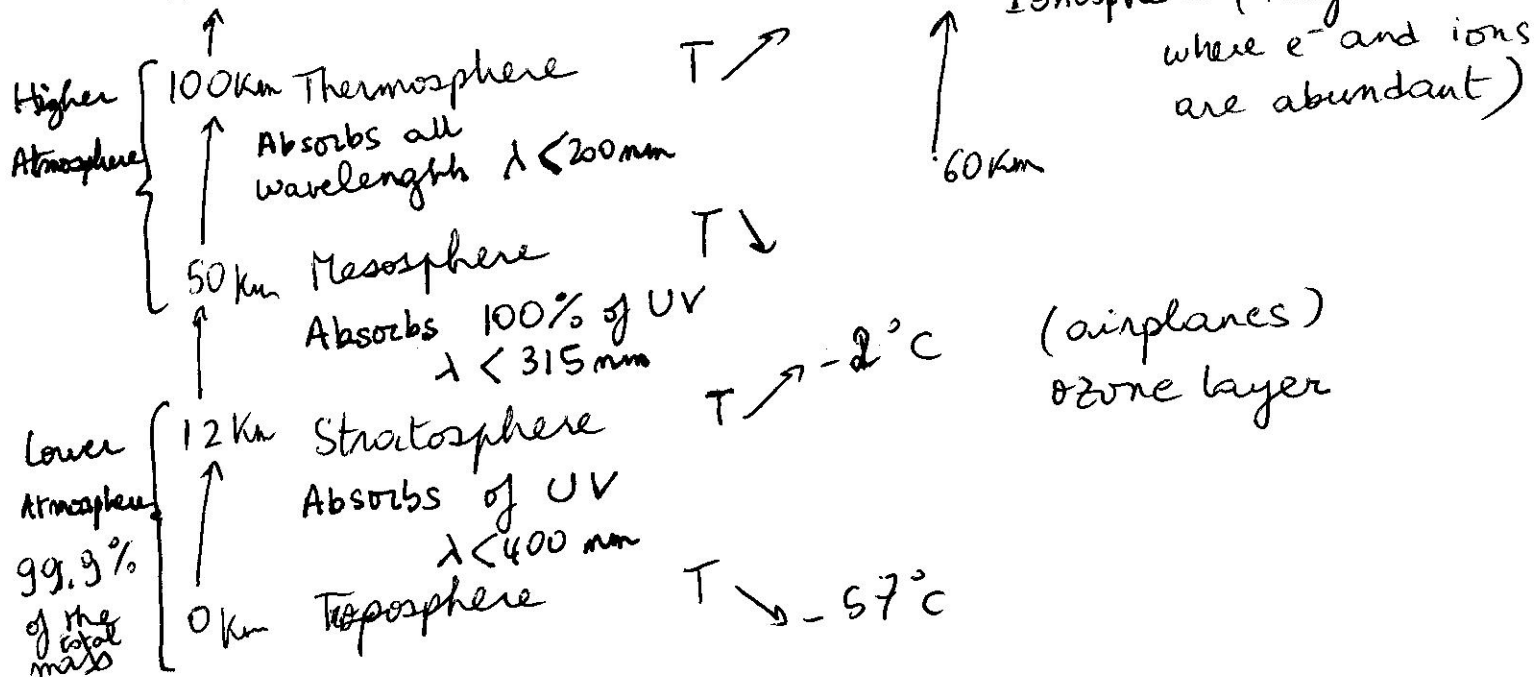
I've taken some of my time to scan my notes and put them on goaub, It is your turn to "loose" 5 minutes of yours!

I hope it was helpful for you!

ENVIRONMENTAL CHEMISTRY

Chapter 1: Atmosphere

ATMOSPHERE



MIXING RATIO

$$x_i = \frac{m_i}{m_{\text{total}}} = \frac{RT}{P} n_i \quad \text{concentration mol/m}^3 \quad n = \frac{m_i}{M_i}$$

(using $PV = nRT$)

Chapter 2: Stratospheric Chemistry

$$P_h = P^0 e^{-\left(\frac{\bar{M}_a g h}{RT}\right)} \Rightarrow \text{Barometric law}$$

P_h → pressure @ h above the sea level in m

\bar{M}_a → ^{avg} molecular weight of air

$$0.02896 \text{ kg mol}^{-1}$$

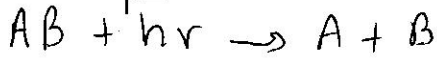
Mass of the atmosphere

$$m_a = \frac{4\pi R^2 P_0}{g}$$

Mass of the atmosphere except the troposphere:

$$m = \frac{4\pi (R+15)^2 P_{h=15}}{g} < m_a$$

example:



$$\Delta H_f = \Delta H_f(A) + \Delta H_f(B) - \Delta H_f(AB)$$

energy

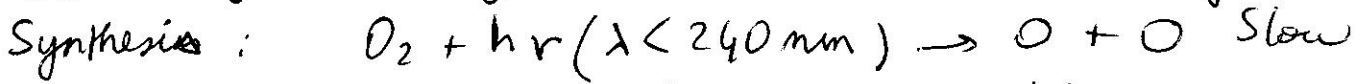
$$\Delta E = h\nu = \frac{hc}{\lambda} \quad (\text{reaction depends of radiation wavelength})$$

1 mole of photon

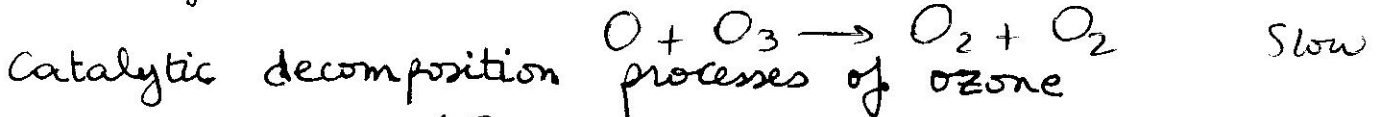
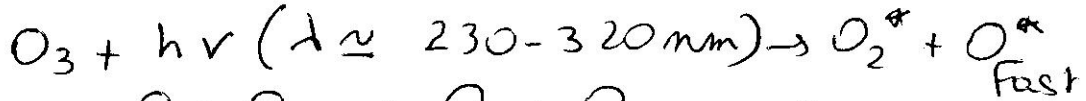
$$\Delta E = \frac{\Delta H_f}{N_A} \quad (\text{for one photon})$$

Free radicals \rightarrow odd number of e^- in a molecule
 $M = \text{catalyst}$

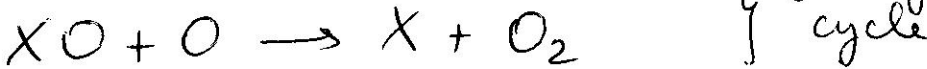
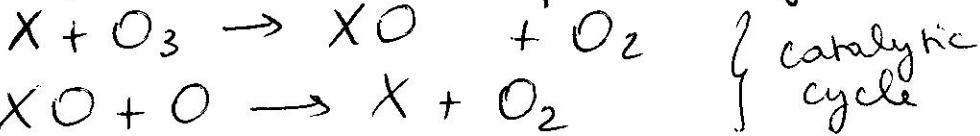
Oxygen-only chemistry - formation and turnover of ozone



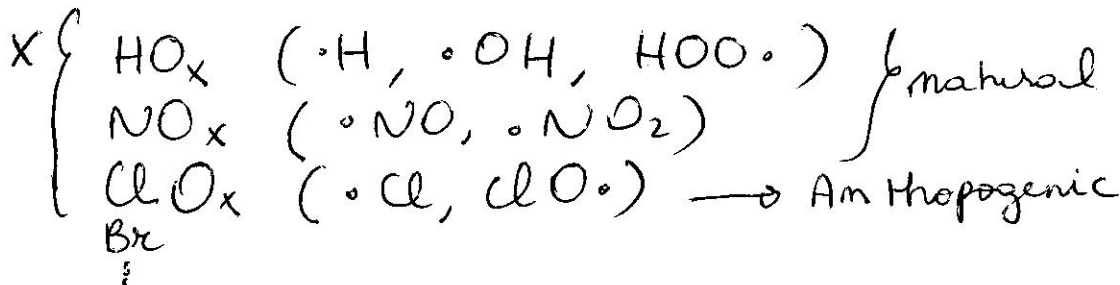
Decomposition:
mill cycle



Catalytic decomposition processes of ozone



} catalytic cycle



CFC - xy_z

$$m_C = x + 1$$

$$m_H = y - 1$$

$$m_F = z$$

m_{Cl} to be found

CFC's undergo UV. decomposition (liberates free radicals) } see holding cycles (reservoirs)

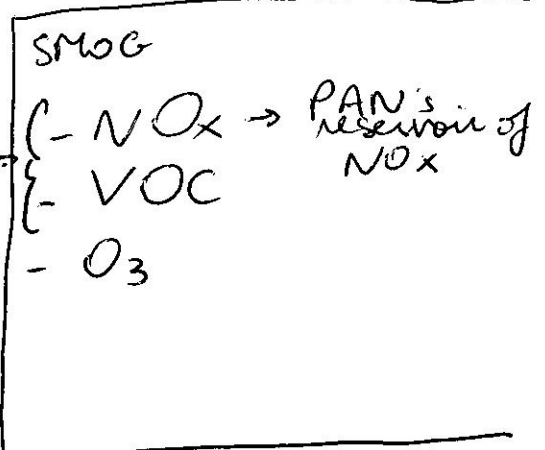
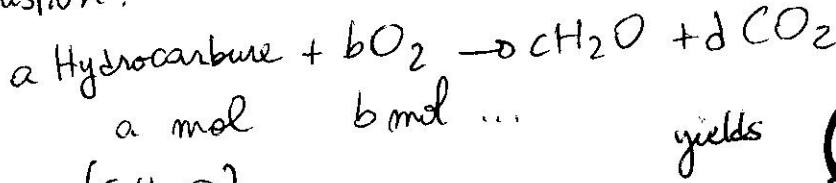
$$k = Ae^{-\frac{E_a}{RT}}$$

Chapter 4: Tropospheric Chemistry

N_2O fertilizer
 NO (nitric oxide)

density $d = \frac{m}{V}$

Combustion:



Hydrocarbon reactivity increases with size and number of double bonds

Biomass: $\{CH_2O\}$
 Gasoline: C_7H_{13}

1 mol air {
 0.78 mol N_2
 0.21 mol O_2
 0.01 mol Ar

Chapter 8: Global Warming

$$m_{atm} = 5.27 \times 10^{18} \text{ Kg}$$

$$\bar{M}_a = 0.02896 \text{ Kg} \cdot \text{mol}^{-1}$$

$$n_{(mol \text{ total})} = \frac{m_{atm}}{\bar{M}_a}$$

→ humidity level in atmosphere

$$P_{actual, H_2O} = \frac{HR}{100} P_v(H_2O)$$

↳ depends of T

↳ $PV = nRT$

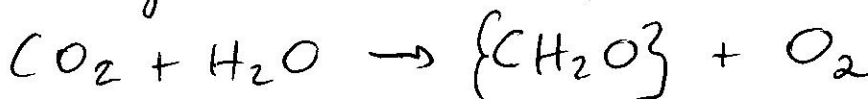
$$F = \sigma T^4$$

↳ Flux (energy emitted from $1m^2$ earth/sun)

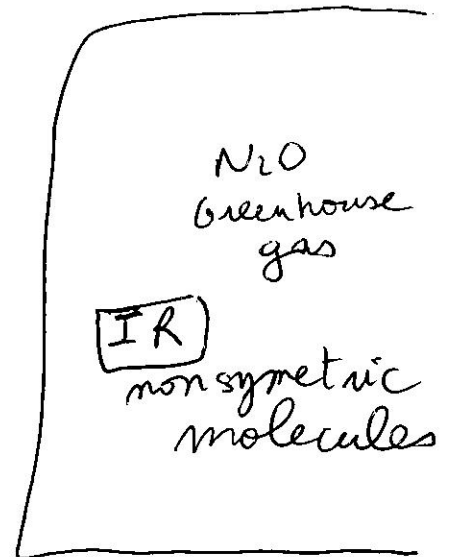
σ : Stefan - Boltzmann constant
 $\sigma = 5.67 \cdot 10^{-8} \text{ W} \cdot \text{m}^{-2} \cdot \text{K}^{-4}$

Chapter 11: Bases in Water

Photosynthesis → biomass



Pure rain: $pH = 5.7$
 Acidic rain: $pH \approx 5.0$



Toxic Metals

Some metals are essential for life
Other are dangerous

$\text{Cr(VI)} \rightarrow$ carcinogen

$(\text{H}_3)\text{Hg}^+ \rightarrow$ toxic

acid pH favorize its formation (lake acidification
would increase mercury toxification)

Cd (similar to Zn)

Hg^0
 Hg_2^{2+}
 Hg^{2+} } non toxic

Biological cycle
(plants, fish, ...)

↓ responsible for
long range transportation
of Hg

Danger: food chain/water

Chapter 11 : Acid Rain

$$pH_{rain} = 5.7$$

acid rain $\rightarrow pH \approx 5.0$

Mass Balance

The mass of acetate (m_{ac}) put into a solution must still be present even though it is now present as HAc and Ac^- .
(same for concentrations).

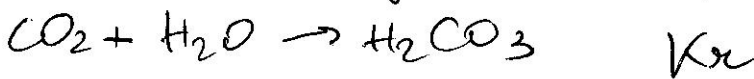
Charge Balance

The total number of positive charges must equal the number of negative charges

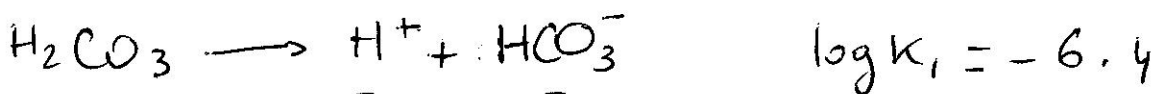
$$[H^+] = [HSO_4^-] + 2[SO_4^{2-}] + [HO^-]$$

To predict how acidic the rain should be

- 1) Estimate how much CO_2 dissolves in the rain to give a solution of H_2CO_3 (use Henry's law P_{CO_2})
- 2) Explore the dissociation of the H_2CO_3 to release H_3O^+



Polyprotic Acid



$$K_1 = \frac{[H^+][HCO_3^-]}{[H_2CO_3]} = 10^{-6.4}$$

$$\Rightarrow \log K_1 = \log \frac{[HCO_3^-]}{[H_2CO_3]} + \log [H^+]$$

$$pK_1 = -\log \frac{[HCO_3^-]}{[H_2CO_3]} + pH$$

$$pH = pK_1 - \log \frac{[H_2CO_3]}{[HCO_3^-]}$$

$$pH = pK - \log \frac{\text{reactive}}{\text{product}}$$

determine predominant species !!

Very Important

$$K_{sp} = [Ca^{2+}][CO_3^{2-}] = 5 \times 10^{-9}$$

\rightarrow to calculate $[Ca^{2+}]$

(solubility product)

Alkalinity (measure of the ability of a water body to neutralize acids)

$$\text{alkalinity} = [\text{OH}^-] + [\text{HCO}_3^-] + 2[\text{CO}_3^{2-}] - [\text{H}_3\text{O}^+]$$

AS $[\text{HCO}_3^-]$
 $[\text{CO}_3^{2-}]$ \rightarrow the solution becomes basic pH \uparrow

\rightarrow To calculate pressure due to water:

Find $V_{\text{H}_2\text{O}} \approx m_{\text{H}_2\text{O}}$
(in liter)

$$F = mg = \text{pressure}$$

\Rightarrow To determine

$[\text{HCO}_3^-]$ and $[\text{CO}_3^{2-}]$

look at the pH and see which species is predominant (other are negligible)

Chapter 16: Water Pollution and Waste Water Treatment

Dissolved oxygen (DO) depends on temperature and altitude

Biological oxygen demand (BOD) = amount of O_2 (in mg) required to carry out the oxidation of organic carbon in one liter of water.

Plant Nutrients: C, N, P = 106:16:1

The shortage of one of these elements keeps the spread of vegetation under control.

Eutrophication = excessive plant growth (algae population explodes)

Primary water treatment (sedimentation process)



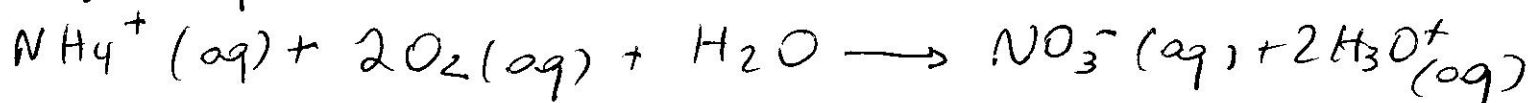
Treatment of phosphorus



Any excess Al^{3+} :

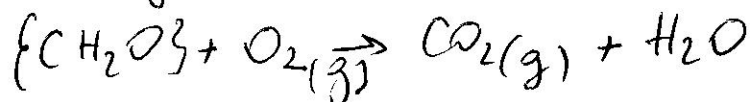


Biological process to remove ammonium

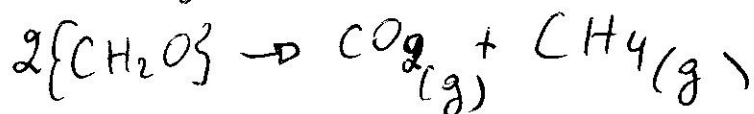


organic matter

presence of O_2 :

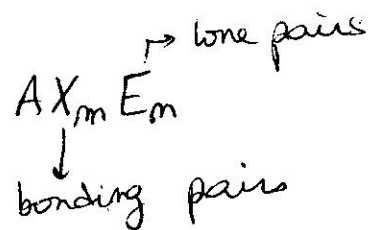


Absence of O_2 :



→ Total carbonate species remains constant (important when we have other reactions)

Molecular Structure : VSEPR



1. Draw the Lewis structure of the atom
2. Count the number of effective pairs (geometry that guaranteed them to be the farthest possible from each other)

e ⁻ arrangement	{	2 pairs → Linear
		3 pairs → Trigonal planar
		4 pairs → Tetrahedral
		5 pairs → Trigonal bipyramidal
		6 pairs → Octahedral

Geometry (depends on X)

AX_4E_0	→ tetrahedral	}	4 pairs of e ⁻
AX_3E_1	→ trigonal pyramidal		
AX_2E_2	→ V-shaped (bent)		
AX_5E_0	→ Trigonal bipyramidal	}	5 pairs
AX_4E_1	→ See-Saw		
AX_3E_2	→ T-structure		
AX_2E_3	→ Linear		

AX_6E_0	→ Octahedral	}	6 pairs
AX_5E_1	→ Square Pyramidal		
AX_4E_2	→ Square Planar		

AX_2E_1 → bent

Chapter 8: Chemical Bonding

Electronegativity (EN) (and ionization energy) \rightarrow Δx
 \uparrow priority
similar to distance from the nucleus to the outer shell (the smallest)

Octet rule (only for the first two periods of the periodic table).

Depicting molecules and ions with Lewis structure:

1. place atom with lowest EN at the center
2. draw single bonds btw atoms after summing the valence e^- and subtract $2e^-$ for each bond from this sum
3. Complete with the remaining e^- (sometimes odd bonds)

When two or more different Lewis structures are possible for a molecule, they are termed resonance hybrid.

Formal Charges = Number of Ve^- in free atom - Number of bonds - Number of nonbonding electrons
(for each atom separately)

In a molecule, we try to obtain the lowest formal charge

ΔE_m = difference in electronegativity (δ^-)
as $\Delta E_m \nearrow$, bonds become more polar
more electronegative (δ^-) |
less electronegative (δ^+)

⚠ Ions

Fe: $[Ar] 4s^2 3d^6$
Fe²⁺: $[Ar] 3d^6$ } because the 4th level ($n=4$) is the outer shell

Size of Atoms

Cu, Cu⁺, Cu²⁺

Cu²⁺ < Cu⁺ < Cu

(less e^- , more attraction)
size = distance from the nucleus to the outer shell

EN(S) < EN(N)

⚠ Elements in period 1, 2
They CAN'T exceed the octet

Most stable Structure

Resonance structures with:

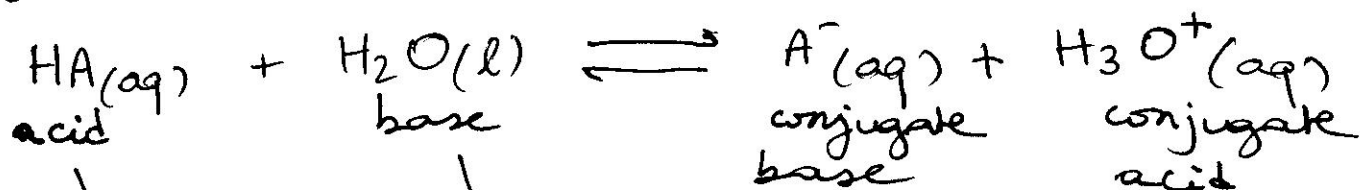
- 1 - lowest formal charges
- 2 - unlike charges on adjacent atoms
- 3 - a more negative formal charge on more E.N. atom

Acids and Bases

Acid: produces hydrogen ions (H^+) in aqueous solution
Base: produces hydroxide (OH^-) ions

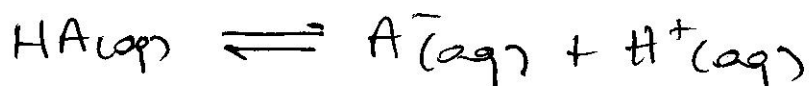


General Reaction



$$K_a = \frac{[H_3O^+][A^-]}{[HA]} = \frac{[H^+][A^-]}{[HA]}$$

K_a is the acid dissociation constant



Strong acid: high K_a (dissociates completely)

Weak acid: low K_a (dissociates partially)

A strong acid yields a weak conjugate base.
(and vice versa)

$$K_w = 1.0 \cdot 10^{-14} \text{ mol}^2/L^2$$

Neutral Solution

$$[H^+] = [OH^-]$$

Acidic Solution

$$[H^+] > [OH^-]$$

Basic Solution

$$[H^+] < [OH^-]$$

$$pH = -\log [H^+]$$

$pH \uparrow$ as $[H^+] \downarrow$

% dissociation is greater in dilute solutions

Polyprotic Acids

Contain more than one acidic proton per molecule.

(H_2SO_4 , H_3PO_4 , H_2CO_3)

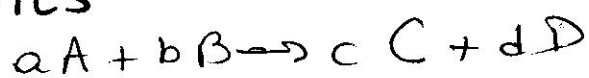
Stepwise dissociation

Only the 1st dissociation step is important in determining the pH

$$K_{a1} > K_{a2} > K_{a3}$$

Only in dilute solutions does the 2nd dissociation step contribute significantly to $[\text{H}^+]$.

CHEMICAL KINETICS



$$\text{Rate} = \frac{\Delta C}{\Delta t} \quad (\text{mol. L}^{-1} \text{ s}^{-1})$$

$$\begin{aligned} \text{rate of reaction} &= \text{rate of disappearance of reactants} \\ &= -\frac{1}{a} \frac{\Delta[A]}{\Delta t} = -\frac{1}{b} \frac{\Delta[B]}{\Delta t} \\ &= \text{rate of appearance of products} \\ &= \frac{1}{c} \frac{\Delta[C]}{\Delta t} = \frac{1}{d} \frac{\Delta[D]}{\Delta t} \end{aligned}$$

Rate law (effect of concentration on reaction rates)

$$r = k [A]^m [B]^n \dots$$

↓
rate constant

0 order reaction:

$$r = k$$

$$m+n+\dots = 0$$

$$[A]_t = [A]_0 - kt$$

1st order reaction:

$$r = k [A]$$

$$t_{1/2} = \frac{\ln 2}{k}$$

$$\ln [A]_t = -kt + \ln [A]_0$$

2nd order reaction:

$$m+n+\dots = 2$$

$$\frac{1}{[A]_t} = kt + \frac{1}{[A]_0}$$

Testing for a Rate law

Plot $[A]$ vs t

$\ln [A]$ vs t

$\frac{1}{[A]}$ vs t

} the straight line \Rightarrow order

Activation Energy

The minimum energy above the average kinetic energy that molecules must bring to their collisions for a chemical reaction to occur.

$$k = A e^{-\frac{E_a}{RT}}$$

↗ activation energy
↘ temperature
↙ perfect gas constant

rate constant ← k
constant ← A

$$\Rightarrow \ln(k) = -\frac{E_a}{R} \cdot \frac{1}{T} + \ln A$$

Slow step followed by fast step

we consider the slow one

Determine
order of reaction?

- initial rates
- graph (straight line?)

Rate Constant?

- slope of line of graph
- formula from graph (rate constant)
- use activation energy

Reaction Mechanisms

(intermediates, balanced equation)

$$r = k[A]^a[B]^b$$

usually,

$$r = k[A][B]$$

Atomic Structure and Periodicity

$$c = \lambda \nu$$

$$c = 3.0 \times 10^8 \text{ m/s}$$

Bohr Model (Valid only for atoms with 1 e⁻)

$$\Delta E = R_H \left(\frac{Z^2}{m_f^2} - \frac{Z^2}{m_i^2} \right) \quad \text{if } m_2 > m_1 \\ \Delta E_2 > \Delta E_1$$

$$R_H = 2.18 \times 10^{-18}$$

$$\Delta E = h \nu = h \frac{c}{\lambda}$$

$$h = 6.6261 \times 10^{-34}$$

Heisenberg uncertainty principle

$$\Delta x \Delta p \geq \frac{h}{4\pi}$$

De Broglie → velocity

$$p = \frac{h}{\lambda} = m v$$

↓
linear momentum

$$\lambda = \frac{h}{m v}$$

Number of orbitals in one atom = m^2

$$l = 0, 1, 2, \dots, m-1$$

$$m_l = -l, \dots, -1, 0, 1, \dots, +l$$

$$m = 1/2, \dots$$

$$m_s = -\frac{1}{2} \text{ or } +\frac{1}{2}$$

$$l = 0 \rightarrow s^2$$

$$l = 1 \rightarrow p^6$$

$$l = 2 \rightarrow d^{10}$$

$$l = 3 \rightarrow f^{14}$$

($2l+1$ orbitals) $\times 2e^-$
in each subshell

Aufbau process (build up and minimize energy)

Pauli exclusion principle (no 2 e⁻ can have all four quantum numbers alike)

Probability of finding an e-
wave function
(Probabilities (0 at nodes))

numb of nodes :

- radial nodes = $n - l - 1$

- angular nodes = l

Total number of nodes = $n - 1$

Done by Erik, VZ.

Save environment!

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