CHEM-101/SA/L01 15/05/23

Refs.

- Essential of Physical Chemistry - Arun Bhal, B.S. Bhal ...
- Inorganic Chemistry, S.2. Haider

Atom

- Evolution of atomic structure
  - Discovery of electron: Cathode rays
  - Discovery of proton: Proton rays
  - " " nucleus: α-ray scattering experiment

Scope of questions that may come

- conclusion of [solar atomic model/...]
- how can we find the nucleus of an atom
- ...

Atom - continuation

- Evo... structure
  - ~~nucleus~~
- ~~limitations~~

Next class: Bor... model

SA/L02 18/05/23

~~Ele~~

~~Bohr model~~

Electromagnetic wave

- perpendicular to each other

Quantum theory

light: discontinuous

$E = h\nu$

Bohr model (1913)

Application: (i) radius of orbit

(ii) Energy of e^- in each ~~sh~~ orbit

(iii) Explanation of hydrogen spectrum

~~Application~~ of Bohr Theory

(i) Position of e^- ~~→ radius of orbit~~

(ii) Energy

(iii) $\Delta E = h\nu$

(iv) $mvr = nh/2\pi$

Application of Bohr Theory

(i) Radius of orbit

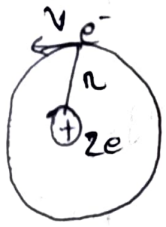
(ii) Energy of electron in each orbit

(iii) Explanation of hydrogen spectrum

Radius of Orbit

Attraction force: $\frac{Ze^2}{r^2}$

Centrifugal force: $\frac{mv^2}{r}$



$$\frac{Ze^2}{r} = mv^2$$

for $Z = 1$,

$$\frac{e^2}{r} = mv^2$$

$$\Rightarrow \frac{e^2}{r} = m\frac{n^2h^2}{4\pi^2r^2m^2}$$

$$\Rightarrow e^2 = \frac{n^2h^2r}{4\pi^2me^2r^2}$$

$$\therefore r = \frac{n^2h^2}{4\pi^2me^2}$$

$$mvr = n\frac{h}{2\pi}$$

$$\Rightarrow v^2 = \left(\frac{nh}{2\pi mr}\right)^2$$

for, $n = 1$

$$r = \frac{h^2}{4\pi^2me^2}$$

$= 0.529 \times 10^{-8}$ cm = Bohr radius

Energy of electron in each orbit

—

K.E + P.E

$= \frac{1}{2} mv^2 + \left(-\frac{e^2}{r}\right)$

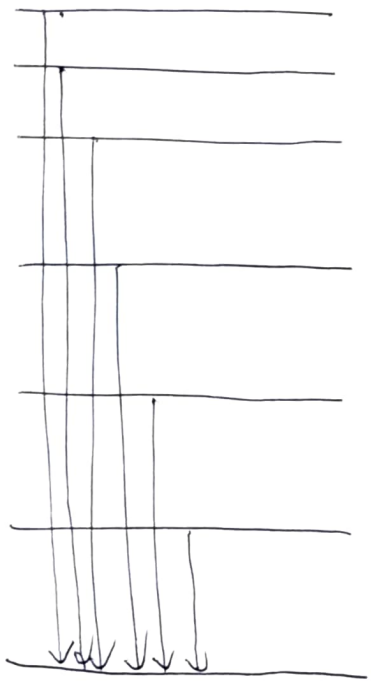
$= \frac{1}{2} mv^2 - \frac{e^2}{r}$

$= \frac{1}{2} \frac{e^2}{r} - \frac{e^2}{r}$

$= -\frac{1}{2} \frac{e^2}{r}$

$\therefore E = \frac{-e^2}{2r} = -\frac{e^2}{2} \times \frac{4\pi^2 m e^2}{n^2 h^2}$

$= -\frac{2\pi^2 m e^4}{n^2 h^2}$



Spectral series of Hydrogen

Series	n_1	n_2	region	wavelength (Å)
Lyman	1	2, 3, 4, 5, 6, ...	Ultra-violet	920 - 1200
Balmer	2	3, 4, 5, 6, 7	visible	4000 - 6500
Paschen	3	4, 5, 6, 7	Infrared	19500 - 18750
Brackett	4	5, 6, 7	infrared	19450 - 40500
Pfund	5	6, 7	infrared	97800 - 75000

Rydberg constant

$$E_{n_1} = -\frac{2\pi^2 m e^4}{n_1^2 h^2}$$

$$E_{n_2} = -\frac{2\pi^2 m e^4}{n_2^2 h^2}$$

$$\Delta E = E_2 - E_1$$

$$= \frac{2\pi^2 m e^4}{h^2}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right] = h\nu$$

$$\Rightarrow h\frac{c}{\lambda} = \frac{2\pi^2 m e^4}{h^2}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

$$\Rightarrow \frac{1}{\lambda} = \frac{2\pi^2 m e^4}{h^3 c}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

$$= R\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

Problems w/ Bohr model

- Heisenberg Uncertainty Principle — violates
- incorrect value for the ground state orbital angular momentum.
- poor predictions regarding the spectra of larger atoms.
- doesn't predict ~~it~~ relative intensities of spectral lines.
- ~~r~~ explain fine structure and hyperfine structure in spectral lines.
- doesn't explain the zeeman Effect.

---

compton, photoelectric

De broglie - Duel nature

$mc^2 = h\nu$

$\Rightarrow mc = \frac{h}{\lambda}$

$\Rightarrow$ mass x velocity $= \frac{h}{\text{wave length}}$

$\Rightarrow$ momentum $= \frac{h}{\text{wave length}}$

Relationship between De Broglie Eqn & Bohrs hypo

$mv = \frac{h}{\lambda}$

$\Rightarrow mvr = \frac{nh}{2\pi}$

$\Rightarrow 2\pi r = n\lambda$

Schrodinger wave equ

$$\frac{\delta^2\psi}{\delta x^2} + \frac{\delta^2\psi}{\delta y^2} + \frac{\delta^2\psi}{\delta z^2} + \frac{8\pi^2 m}{h^2}(E-V)\psi = 0;$$

ψ : wave function

ψ^2 = aplitude of the probably of finding e^- in a 3d space.

$H(\psi) = E(\psi)$

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Quantum Numbers

1. Principle Quantum Number
2. Azimuthal
3. Magnetic
4. Spin

imp for CT
d orbital diagram

Principle.

Azimuthal ...

- s orbital — sharp — spherical [⊗]

  p orbital — principle — dumbbell [∞]

  d " — diffused — Clovenleaf

  f " — fundamental — too complex

Magnetic ...

- $f_{xyz} = f_{x(x^2-3y^2)}$, f_{xz^2}, f_{yz^2}, $f_{z(x^2-y^2)}$

  f_{z^3}, f_{xy^3}, $f_{y(y^2-3z)}$

Spin...

- $+\frac{1}{2}$: anti-clockwise
- $-\frac{1}{2}$: clockwise

Electron configuration of a atom

- Pauli Exclusion principle
  - states the maximum number of e^- that can ~~sat~~ stay in a shell.
- Aufbau principle

$$\frac{1}{\lambda} = R_H \left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

$$\therefore \lambda = \left[109678 \left[\frac{1}{2^2} - \frac{1}{3^2}\right]\right]^{-1}$$

$$= 6564.79 \text{ Å}$$

$N, K^+, Ne, S, Cl^-, Cu^{+}, Sc$

four quantum numbers of last electron

Four quantum numbers of the last electron of:

N: [He] $\boxed{\uparrow\downarrow}$ $\boxed{\uparrow}\boxed{\uparrow}\boxed{\uparrow}$

2s 2P

$n = 2$

$l = 1$

$m = 1$

$s = +\frac{1}{2}$

K^+: [Ne] $\boxed{\uparrow\downarrow}$ $\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}$ $\boxed{\ }$

3s 3p 4s

$n = 3$

$l = 1$

$m = 1$

$s = -\frac{1}{2}$

Ne: [He] $\boxed{\uparrow\downarrow}$ $\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}$

2s 2P

$n = 2$

$l = 1$

$m = 1$

$s = -\frac{1}{2}$

S: [Ne] $\boxed{\uparrow\downarrow}$ $\boxed{\uparrow\downarrow}\boxed{\uparrow}\boxed{\uparrow}$

3s 3P

$n = 3$

$l = 1$

$m = -1$

$s = -\frac{1}{2}$

Cl^-: [Ne] $\boxed{\uparrow\downarrow}$ $\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}$

3s 3p

$n = 3$

$l = 1$

$m = 1$

$s = -\frac{1}{2}$

Cu^{2+}: [Ar] $3d^{10}\ 4s^1$

Cu^{2+}: [Ar] $3d^9\ 4s^0$

$n = 3$

$l = 2$

$m = \pm 1$

$s = -\frac{1}{2}$

Sc: [Ar] $3d^1 4s^2$

$n = 4\ 3$

$l = 0\ 2$

$m = 0\ -2$

$s = +\frac{1}{2}$

SA 01/06/23

Chapter review

1. α-particle, α-particle scattering exp, conclusion, Rutherford solar system model, limitation,

2. Quatum theory of light – Max Planck,

3. Bohr model, applications

a) Derivation of the equ. to determi...
R.E.

b) Atomic of hydrogen

c) Rhydberg const

4. Dual nature of electron

$$n\alpha\frac{1}{\lambda}$$

$$2\pi r = n\lambda$$

5. Heisenberg uncertainty principle

6. Schrondinger equation

ψ, ψ^2 significance

7. Quantum numbers

a) Electron configuration

Pauli

Aufbauf

Hunde

Chapter 2/ Periodic Table

Mendeleef's periodic table & law

Modern " "

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08/06/23

Classification of elements

1. Inert gas
2. Representative elements
3. Transition metal
4. Inner-transition

Transition metal

- Catalytic property

Periodicity (def)

Variation of properties within

- metallic char (down)
- Atomic radius
- Electro af

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Limitations of periodic table

1. Position of Hydrogen
2. Anamolies in the Mandeleeff Table
3. Position of Lathanide and Actinides
4. Position of isotopes.
5. Diagonal relation

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1. Periodic law
   a) mandleef
   b) Modern
2. Features of periodic table
3. Classification of elements according to periodic law.
4. Periodicity
5. Valency of an atom is periodic function of or it is not.
6. Variation of different atomic properties in periods & groups
   - atomic stuff
   - Electronegativity
   - IP/EE

7. Periodic table limits

Nobel gas

- discovery
- physical props
- chemical props

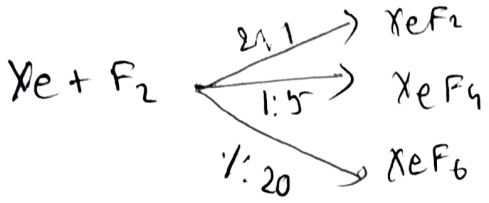
why called inert

- Doublet / Octant
- I.E. very high
- Electron affinity very low

Ar, Kr, Xe → 3d exist

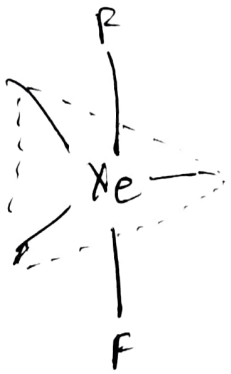
∴ coordinating

XeF_2 XeF_4 & XeF_6 formation



Compound of inert gases

Geometric structure



Uses of inert gas

Sample ques: 3 usages of Neon

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Arrhenius concept

$HCl_{(aq)} \rightarrow \underline{H^+} + Cl^-$

acid

$NaOH_{(aq)} \rightarrow Na^+ + \underline{OH^-}$

base

limits

i) aq. medium

ii) not all bases release base

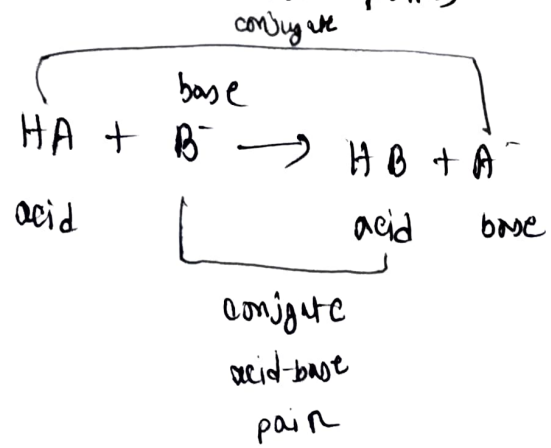
iii) ...

Bronsted - Lowry concept

acid → donates proton (H^+)

base → accepts proton &

Conjugate Acid-base pairs



acid strong → base weak

base " → acid "

Amphiprotic substance : behaves both like acids & bases.

Lewis concept of acids and bases

acid → e pair acceptor ; usually cations

base → e pair donor ; " anions

Auto ionization of water

Relative strength of acids

H_3AsO_3 → 3

H_2SO_4 → 6

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

$\Rightarrow [H^+] = 10^{-pH}$

Development of pH scale and pH of pure water

$$H_2O \rightleftharpoons H^+ + OH^-$$

$$K = \frac{[H^+][OH^-]}{[H_2O]}$$

$\Rightarrow K \times [H_2O] = K_w = [H^+][OH^-]$

$= [H^+][H^+] \quad \because [H^+] = [OH^-]$

$= [H^+]^2$

$\Rightarrow 1 \times 10^{-7} = [H^+]^2$

$\Rightarrow [H^+] = 1 \times 10^{-7}$

$\Rightarrow -\log([H^+]) = -\log(1 \times 10^{-7})$

$\therefore pH = 7$

$[H^+] = [OH^-] \rightarrow pH\ 7$

$[H^+] > [OH^-] \rightarrow pH < 7$

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

$pOH = -\log [OH^-]$

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

$-\log(K_w) = -\log[H^+] - \log[OH^-]$

$pK_w = pH + pOH$

$\Rightarrow 14 = pH + pOH$

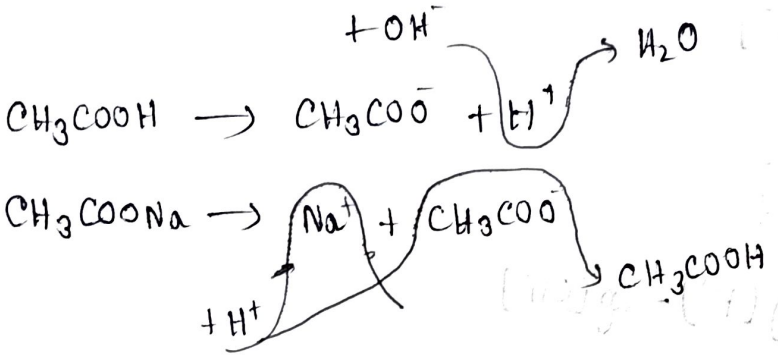
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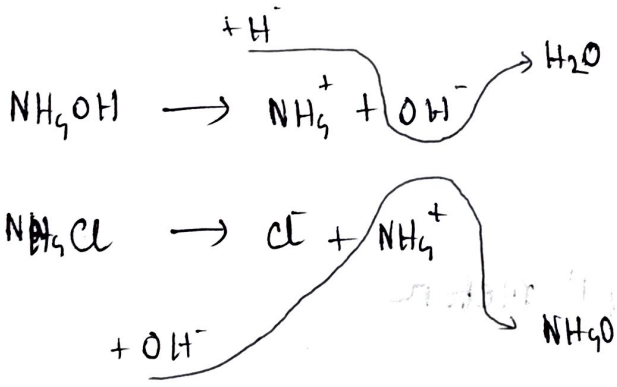
pH measurements / pH meter

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Buffer solution





Handerson - Hasselbalch equation

$$HA \rightleftharpoons H^+ + A^-$$

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

[HA] = init concentration

$$HA \rightarrow H^+ + A^-$$

$$ANa \rightarrow Na + A^-$$

$$pK_a = pKa + \log \frac{[salt]}{[acid]}$$

pH

Equivalent point

End point

Methyl orange

Methyled ⟶ red-orang

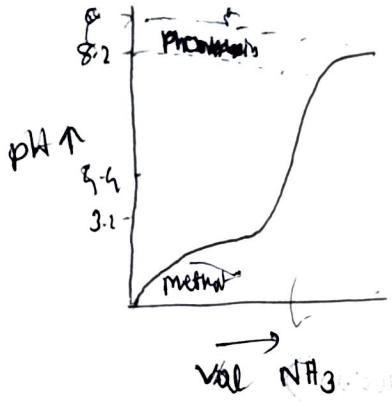
Litmus

Bromothymol blue

Phenolphathalein

pH curve and indicators

(a) weak acid & strong base



—

Theories of Acid-base indicators

The Ostwald's theory

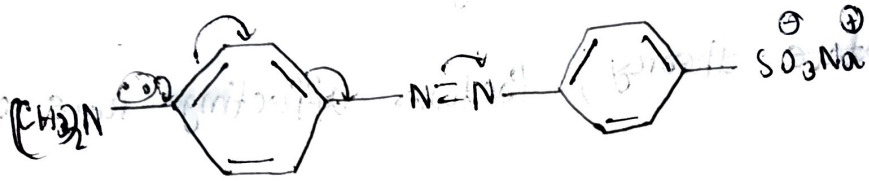
$HIn \rightleftharpoons H^+ + In^-$

$K_{in} = \frac{[H^+] + [In^-]}{[HIn]}$

yellow !

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Methyl Orange / Indicator



Base

Acid

$(CH_3)_2N$

Phenolphthalein

Acid Rain

Mathes

Find out the pH of a

From Text books

Chemical Bond

Valence e⁻

Non-bonding e⁻

Types of Bond

i) Ionic bond / Electrovalent bond

ii) Covalent bond

iii) Coordinate bond

Ionic :

Conditions for formation of ionic bond

- Number of valence electrons
- Net lowering of energy
- Electronegativity difference

Factors governing the formation of ionic bond.

-

Ionic bonds form lattic

-

Characteristics of ionic compounds

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10/07/2023

Covalent Bond

- Characteristics

Coordination bond

Polarn covalent bond (

A covalent bond in which electrons are shared unequally and the bonded atoms acquire a partial positive and negative charge, is called a polar covalent bond.

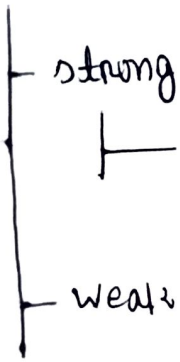
Hydrogen bond

Types of it

Characteristics

Metalic bond

Chemical bonding

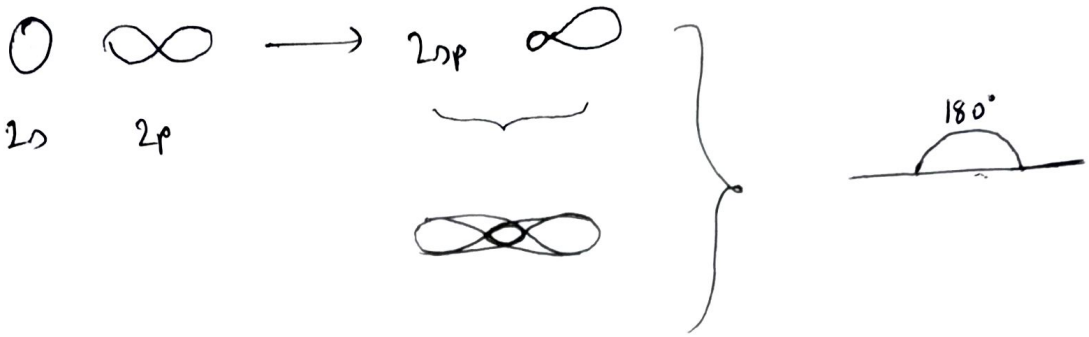


SA 24/07/23 $t_{1/2} = \frac{\ln 2}{k}$ $\ln[A]_t = -kt + \ln[A]_0$

VBT

Hybridization

sp hybridization



(structure geometry shape)

$sp \rightarrow sp^3d^3$

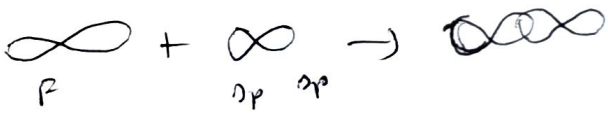
BeF$_2$

$Be: 1s^2 2s^2 2p_x 2p_y 2p_z$

$Be^*: 1s^2 2s^1 2p_x^1$

$O + \infty = \infty$

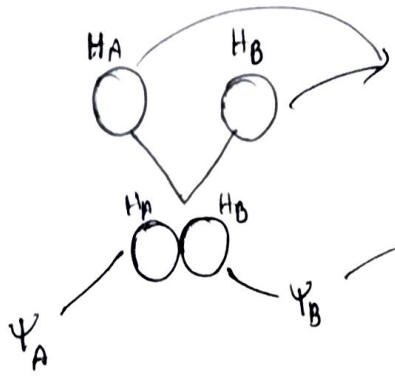
F = ...



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Molecular Orbital Theory

Linear Combination of Atomic orbitals (LCAO method)



s orbital: H atom

wave func.

bonding → +,+ / −,−

anti-bonding → +,−/

σ, π

σ*, π*

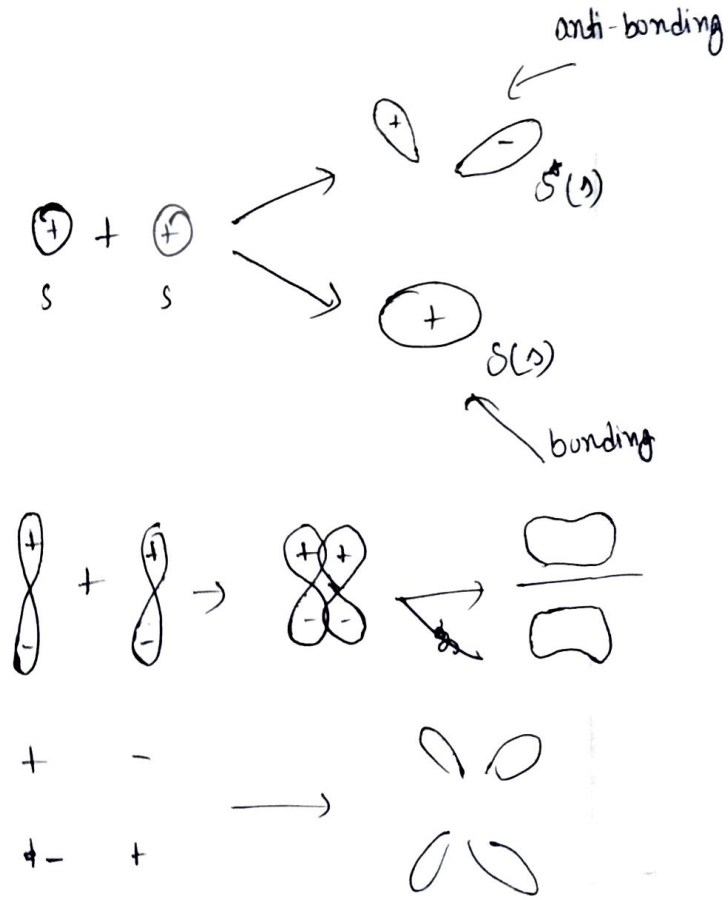
$\Psi(MO) = \Psi_A \pm \Psi_B$

Possible combinations:

~~s + s~~

~~s + p~~

~~p + p~~



Conditions

$s - s \rightarrow$ sigma

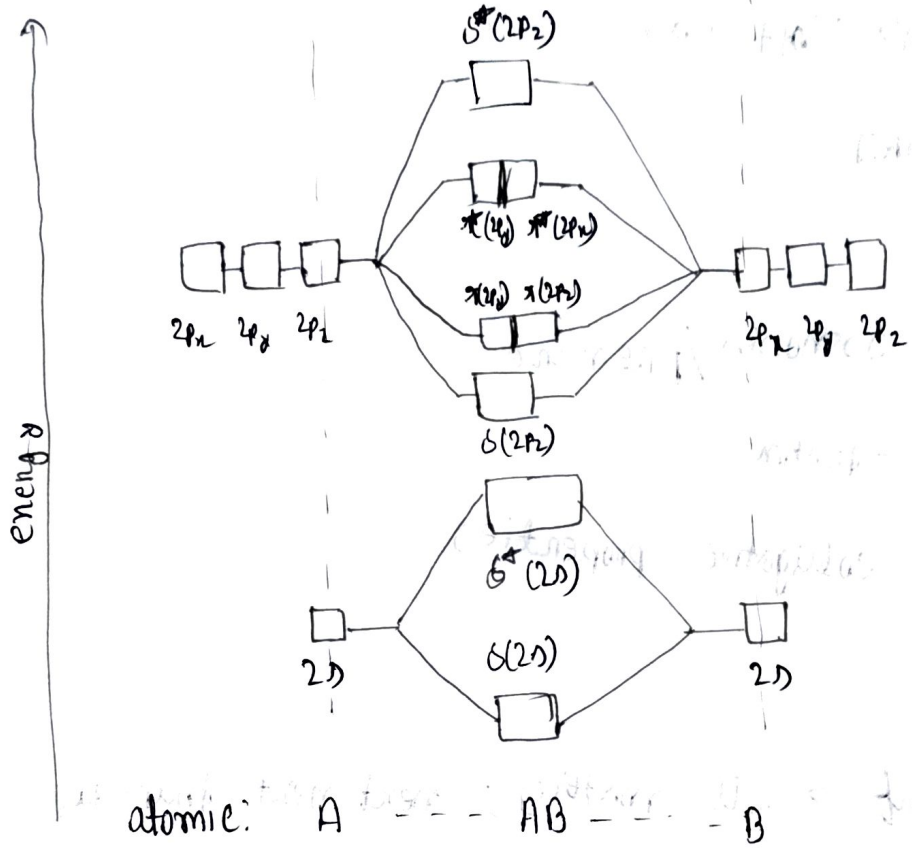
$s - p_z \rightarrow$ sigma

$p_z - p_z \rightarrow$ sigma

$p_y - p_y \rightarrow \pi$

$p_x - p_x \rightarrow \pi$

Energy of Molecular orbitals



atomic: A --- AB --- B

atomic orbital — atomic orbital

~~$\sigma(1s)\ \sigma^*(1s)$~~

~~$\sigma(1s)\ \sigma(2s)$~~

$\sigma(1s)\ \sigma^*(1s)\ \sigma(2s)\ \sigma^*(2s)$ ---

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31/07/23

Bond order

Molecular diagram of H_2

① atom e⁻ config

② diagram

③ molecular e⁻ config

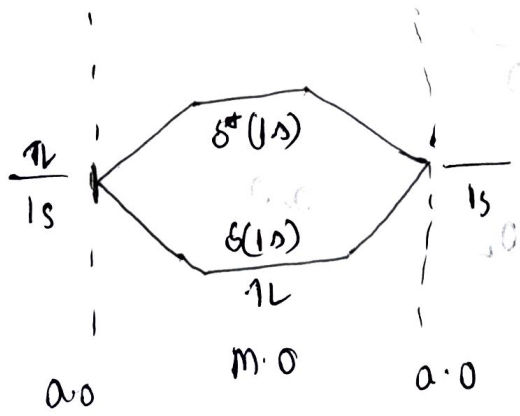
④ bond order

⑤ magnetic props

---

② →

H_2



$H_2 = \sigma(1s^2)\ \sigma^*(1s^0)$

B.O $= \frac{2-0}{2} = 1$ | $\frac{\text{Bonding} - \text{anti}}{2}$

B.

He_2

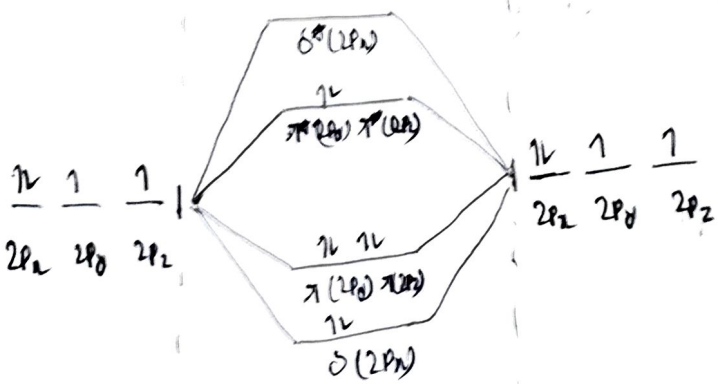


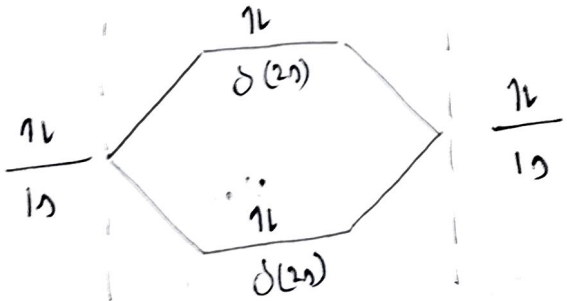
B.O $\frac{2-2}{2} = 0$; doesn't exist

Ne : $1s^2 \boxed{2s^2\ 2p^6}$

O : $1s^2\ 2s^2\ 2p_x^2\ 2p_y^1\ 2p_z^1$

O_2 :





a.o MO of O_2 a.o

H.W

CN / Molecular orbital

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07/08

Organic Chem — Reaction mechanism

Source:

1. Plants & animals
2. Natural gas & Petroleum
3. Coal
4. Fermentation
5. Synthesis

Classification:

1. Aliphatic
2. Aromatic
3. Alicyclic
4. Heterocyclic

Functional group.

Alkane	$-C-C-$	Ethane	H_3C-CH_2
Alkene	$>C=C<$	Ethene	$H_2C=CH_2$
Alkyne	$-C\equiv C-$	Ethyne	$HC\equiv CH$
Alcohol	$-OH$	Ethanal	H_3C-CH_2-OH
Acid	$-COOH$	Ethanoic acid	$H_3C-COOH$
Amine	$-NH_2$	Ethylamine	$H_3C-CH_2-NH_2$
Halo Alkyl	$-X$	Ethyl	

Substitution

Addition

Elimination

Oxidation & Reduction

Polymerization

Degrees → 1°, 2°, 3° C

Stability of Carbocation

carbanion

reactant + attacking group

- Electrophilic: H^+, X^+, R_3C^+
- Nucleophile: Cl^-, Br^-, X^-, OH^-, CN^-, NH_3, H_2O

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① Substitution

↓

Free radical. — (a)

Electrophilic — (b)

Nucleophilic — (c)

(a) $CH_4 + Cl_2 \xrightarrow[50^\circ]{UV} CH_3Cl + HCl$

Step 1: Initiation

$Cl_2 \xrightarrow{h\nu} 2Cl^\cdot$

Step 2: propagation

$CH_4 + Cl^\cdot \longrightarrow CH_3^\cdot + HCl$

$CH_3^\cdot + Cl_2 \longrightarrow CH_3Cl + Cl^\cdot$

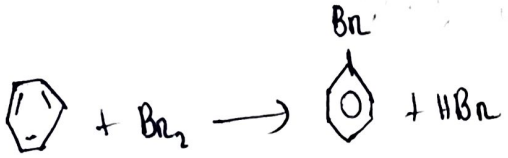
Step 3: Termination

$Cl^\cdot + Cl^\cdot \longrightarrow Cl_2$

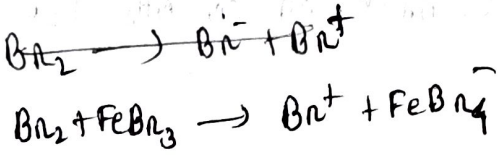
$CH_3^\cdot + Cl^\cdot \longrightarrow CH_3Cl$

$CH_3^\cdot + CH_3^\cdot \longrightarrow CH_3-CH_3$

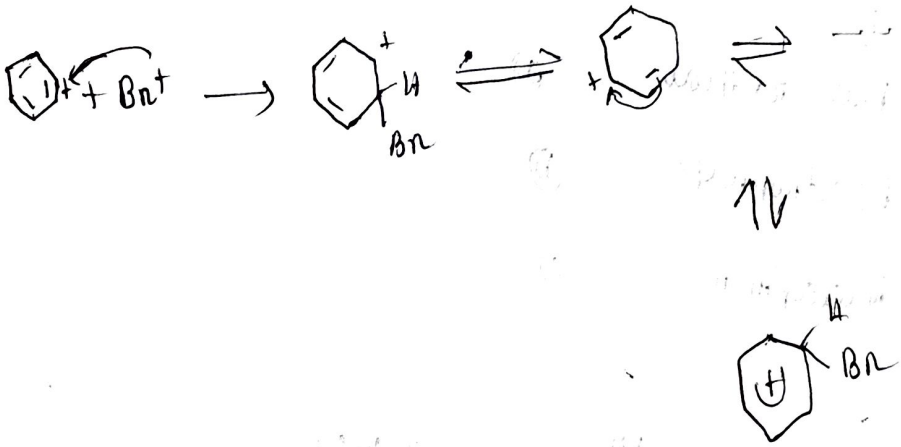
(b)



Step 2: Formation of electrophile



Step 2:



Step 3



Nucleophilic Substitution : S_N1, S_N2

Unimolecular Nucleophilic Substitution

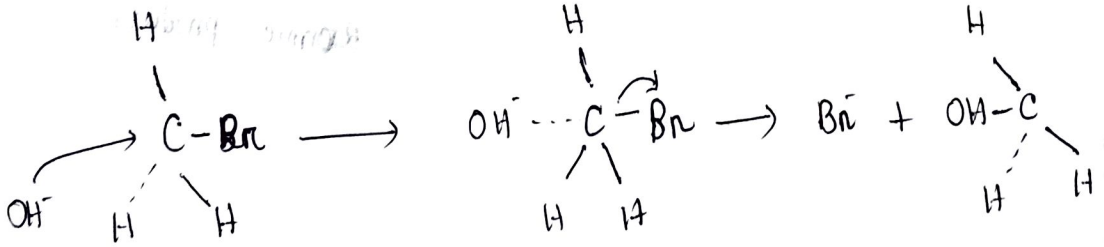
Bimolecular

$R_3C-X + OH^- \longrightarrow R_3C-OH + X^-$

Rate = K[Alkyl halide]

Rate = K[alkyl halide][attacking/alcohol]

S_N2



transition state

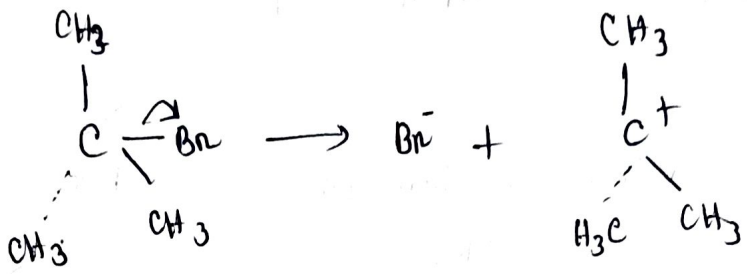
Inversion of product

Inverted product

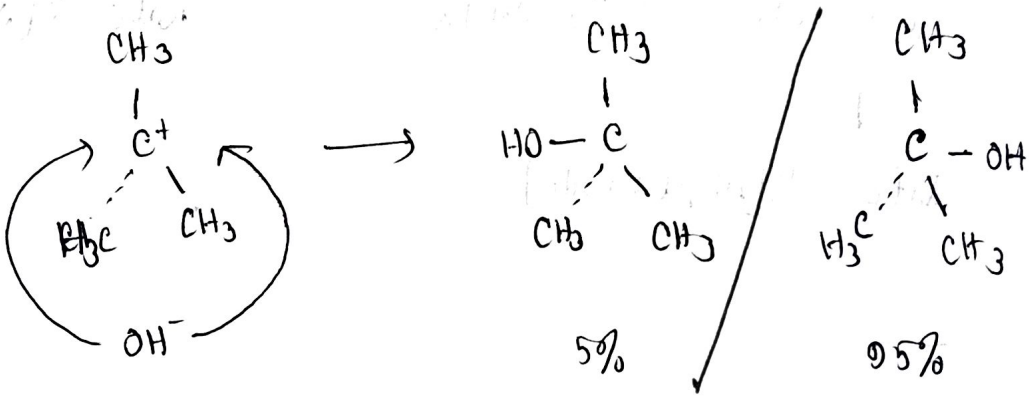
Walden Inverse

S_N1

1st step:



2nd step:



Racemic product

which mechanism to follow:

Factor affect SN

(I) Strong Nucleophile → Strong follows SN2

(II) Structure of Alkyl Halide → Carbocation
→ steric hindrance

(III) Having group

(IV) Solvent — Protic → SN_1
Aprotic → SN_2

Addition reaction

$>C=C<$ } electrophilic addition

$>C\equiv C<$ }

$>C=O$ } Nucleophilic addition



$>C=\ddot{O}$

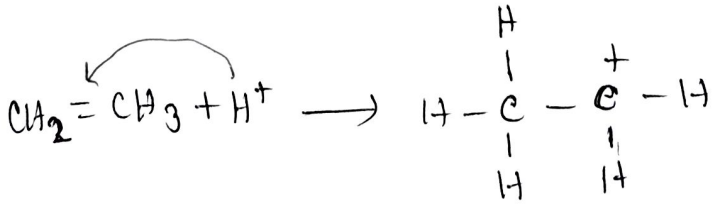
$>C^{\delta+}\cdots\ddot{O}^{\delta-}$

Nucleophilic

$CH_2=CH_2 + HBr \longrightarrow CH_3-CH_2Br$

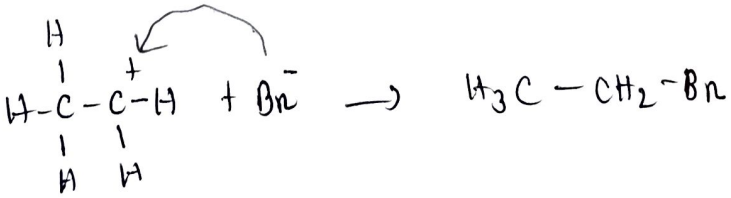
step 1 : $H-Br \rightarrow H^+ + Br^-$

step 2 :

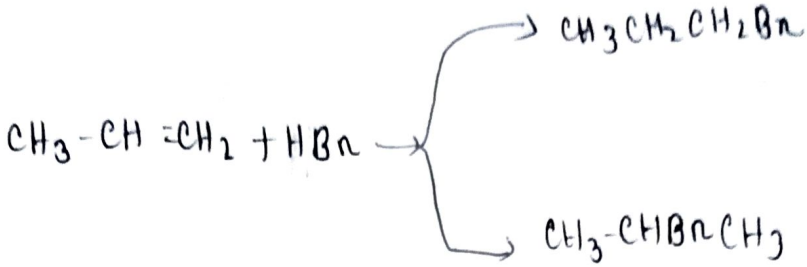


$CH_2=CH_3 + H^+ \longrightarrow$ H–C(H)(H)–C$^+$(H)–H

step 3 :

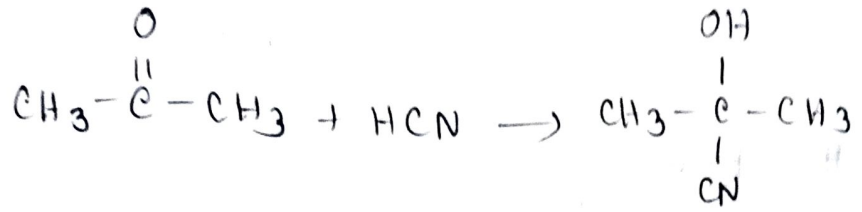


H–C(H)(H)–C$^+$(H)–H + Br^- $\longrightarrow$ H_3C-CH_2-Br



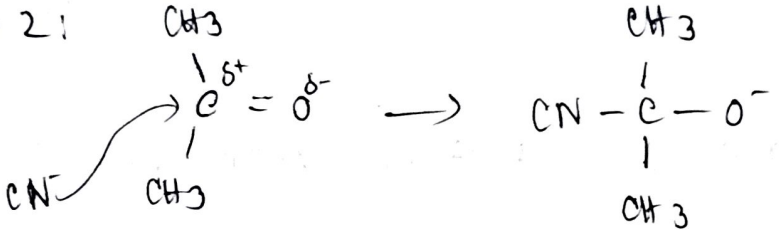
(90%: Markovnikov's law due to the stability of carbocation

Anti-Markovnikov's law + H_2O_2 then reverse prod.

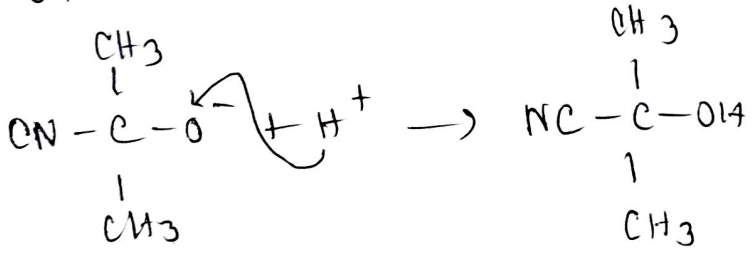


step 1 : $HCN \rightarrow CN^- + H^+$

step 2 :



step 3 :



Elimination Reaction

[~~deeper~~ mechanism can be skipped for final]

$$R-CH_2-CH_2-X \xrightarrow{OH^-} R-CH=CH_2 + H_2O + X^-$$

Unimolecular E_1

Bimolecular E_2

CHEM 101 / SA

16/08/23

1. Chap 1: Atomic structure

1. α-particle, x-ray scattering exp., conclusion, Rutherford model, limitation

2. Bohr model & limitation.

3. a) Radius eqn derivation

   b) Energy eqn "

   c) Rydberg constant calc

   d) H-spectre + math

4. Dual nature, $2\pi r = n\lambda$

5. Heisenberg theory (just theory)

6. Schrodinger eqn., significance of ψ, ψ^2
   - ψ → no physical significance; ampli...
   - ψ^2 → direct physi... sig.

7. Quantum numbers significance

8. Pauli, Hund, Aufbaul principle

9. Electric config

Periodic table

1. Periodic law
2. Classification of elements based on e^- configuration
3. Periodicity.
4. Properties in periods & groups.
5. Limitations

Inert gas

1. Reason of inert
2. Compounds, uses (2, to 3)

1. Defⁿ of covalent, ionic bond, coordinate

2. Condition, characteristics

3. Polar covalent

4. H-bond, types, H-bond characteristics

VBT + VSPER

1. Defⁿ

2. σ, π bond

3. Hybridization defⁿ.

4. sp, sp^2, sp^3, dsp^3, d^2sp^3, dsp^2

★★★ 5. $BeCl_2$ [Hybridization + apply VSPER theory]

MOT

1. Defⁿ

2. LCAO

3. B.O & A.B. orbitals

4. Bond order, significance

★★★ 5. Molecular orbital diagram → Magnetic prop, stability ...

Acid - base

1. Different concepts

2. H_2O amphoteric

3. pH, pH determination

   ① Indicator

   ⑪ pH meter

4. Relation between pH & pOH

5. Buffer, types of buffer Buffer mechanism, common ion effect.

6. Derivation Hendeson eq^n, significance

7. pH titration curve. (S.A & S.b, S.A & W.b, W.A, S.b)

Organic chem

Everything from class notes + carbonizing. --

☆☆ Nucleophilic mechanism & factors

Additive reaction

☆☆ the makinov's rule

~~Elimination~~ X