CHEMISTRY

3rd class Date : 20-09-2021

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Last class…

- General introduction – Course

General information, 21CYB101J

- **6 classes / week** (I day order : 9.00 – 10.40 am, III day order : 10.50 – 11.40 am, V day order : 1.20 – 2.10 pm. ***5 credit course*** (incl. 2 lab class). Lab. : III day order : 2.10 – 3.50 pm
- **Location and contact**: Virtual classroom (Google Meet), mobile and email.
- **Activities**: Teach the entire syllabus, provide lecture material as hand outs, announce assignments, take laboratory sessions & conduct CLA's, end semester.
- **Grading/weightage:** Assessment test I – 15%, Assessment test II – 15%, Assessment test III – 20% & Assignments – 10%, End Semester – 40%.

General information, 21CYB101J

- Kindly join 1-2 minutes prior to the start of the session
- Attendance – 'in' and 'out' times are recorded automatically
- Please choose "join Meeting" and do not choose "present" in the meeting option
- As you join the session, **kindly mute your audio and video**
- If you have any queries, please unmute yourself and ask or type in the chat box !
- If the internet is disconnected (or any issues on my side), please alert me !

Preface, 21CYB101J

- Syllabus – following AICTE norms, first time at SRMIST !!
- Refer SRMIST curriculum
- Weightage : Both theory and lab.
- Continuous learning assessment (CLA) pattern
- Attendance (minimum 75% is a must)

Preface, 21CYB101J

- The contents of the slides will not deviate markedly from the usual textbooks. (Other reference material if any will be provided).
- Effort will be made to present as much visual information as possible and make the class more interactive.
- Important slides will be marked with a "***X***" *symbol* in one of the corners of the slide.
- The entire course material is intended for learning and understanding of the subject matter (not merely for 'exams' or 'syllabus coverage').
- Lecture slides, notes and handouts will be provided in a regular basis ***(Google Classroom)***

X

Reference text books, 21CYB101J

- B. H. Mahan, R. J. Meyers, University Chemistry, 4th ed., Pearson publishers, 2009.
- Peter W. Atkins, Julio de Paula, James Keeler, Physical Chemistry, 11th ed., Oxford publishers, 2018
- W. D. Callister, D. G. Rethwisch, Materials Science and Engineering: An Introduction, 8th ed., Wiley, 2009
- M. J. Sienko, R. A. Plane, Chemistry: Principles and Applications, 3rd ed., McGraw-Hill publishers, 1980

Goals & purpose

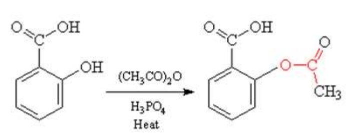
- Brief introduction to concepts in chemistry (level 2 hybrid undergraduate course)
- Utilize concepts in chemistry for technological advancement based on atomic and molecular level modification
- This course will help you as an engineer to:

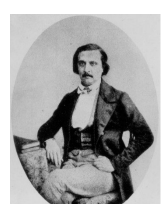
1) Fundamental understanding of concepts
2) Importance of chemistry in various technological applications and in industries
3) As a M.Tech (Int.) student : 5 credits, good for CGPA ☺

What is Chemistry?

- The study of matter (composition, structure, properties, changes,……)
- Science → Pure (Knowing)
  - Does not necessarily have an application
- Technology → Applied (Doing)
  - Has practical applications in the society, **engineering**
- **Interdisciplinary field** : Material chemistry, pharma, agro, engineering etc. Everything we see and use is made from materials : metals, polymers, ceramics, semiconductors and composites (**basis set is chemistry**)

Science to Technology?





Charles Frédéric Gerhardt

Science to Technology?

- Fuselage (A350) is built with **carbon-fibre reinforced plastic (CFRP)** – which supports lower fuel burn, easier maintenance and increased resistance to corrosion.

Science to Technology ?

Syllabus overview

Total FIVE chapters

- ❑ Inorganic chemistry
- ❑ Physical chemistry
- ❑ Organic chemistry
- ❑ Polymers
- ❑ Advanced engineering materials

Inorganic chemistry

- ❑ Coordination complexes, introduction
- ❑ Crystal field theory : different complexes, low and high spin, magnetism and optical properties
- ❑ Periodic properties : Slater's rule, electronic configurations
- ❑ Variation in periods and groups : Size, electronegativity, ionisation energy & electron affinity
- ❑ HSAB principle

Physical chemistry

- Thermodynamics : U, Q, W, T, H, S, ΔG, Gibbs-Helmholtz equation
- Electrochemistry : Nernst equation, Applications
- Corrosion : Types, Pourbaix diagram
- Chemical equilibrium and solubility product

Organic chemistry

- Isomerism : Structural, Configurational and Conformational
- Absolute configuration : CIP rules (naming enantiomers)
- Conformational analysis
- Reactions : Substitution, Elimination, Oxidation, Reduction, Addition, Cyclisation and C-C bond formation reactions
- Synthesis of pharmaceutical products, few examples

Polymers

- Introduction to concept of macromolecules - Classification of Polymers
- Types of Polymerization - Important addition and condensation polymers
- Synthesis and properties – Polypropylene, polystyrene, PVC, Teflon, Nylon, PET, Polyurethane and Synthetic rubber
- Conducting polymers – introduction, types

Advanced engineering materials

- Mechanical properties of solid – stress-strain relationship
- Tensile strength, Hardness, Fatigue, Impact strength, Creep
- Composite materials - introduction and types (FRC, MMC, CMC) – Applications
- Surface characterisation techniques - XRD and XPS

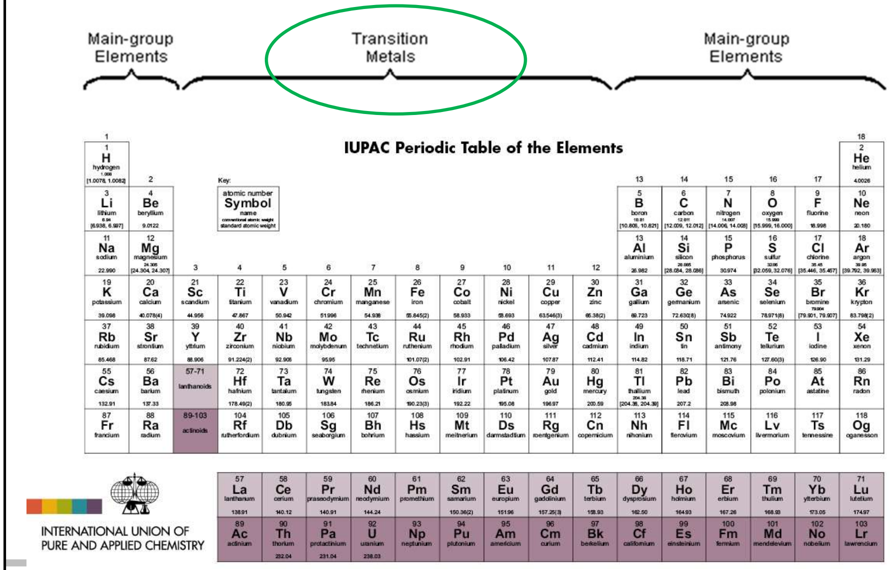
Summary, CLR

- Exploit the periodic properties of elements for bulk property manipulation towards technological advancement
- Address concepts related to electrochemistry, such as corrosion, using thermodynamic principles
- Employ various organic reactions towards the design of fine chemical and drug molecules for industries
- Brief outline, reaction types and applications of polymers
- Properties, surface characterization and applications of advanced engineering materials
- Utilize the **basic chemistry principles** applied in various engineering problems and identify appropriate solutions

Chapter 1, contents

- Coordination complexes – introduction
- Crystal field theory : different complexes, low and high spin, magnetism and optical properties (coordination complexes)
- Slater's rule, electronic configurations
- Variation in periods and groups - Size, electronegativity, ionisation energy & electron affinity

Coordination compounds



Coordination compounds

- **Main group elements -** the valence electrons of the isolated atoms combine to form chemical bonds that satisfy the octet rule. The one valence electron leaves sodium and adds to the seven valence electrons of chlorine to form the ionic formula unit NaCl.

- Transition metals do not normally bond in this fashion. ***They primarily form coordinate covalent bonds,*** a form of the **Lewis acid-base** interaction in which **both of the electrons in the bond are contributed by a donor (Lewis base) to an electron acceptor (Lewis acid).**

- The Lewis acid in coordination complexes, often called a central metal ion (or atom), is **often a transition metal or inner transition metal**

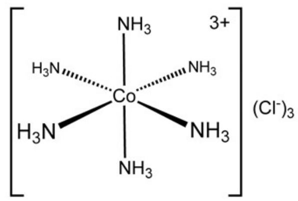
- The Lewis base donors, called **ligands**, can be a wide variety of chemicals—atoms, molecules, or ions.

- ***The only requirement is that they have one or more electron pairs, which can be donated to the central metal.***

Coordination complex

- Species where transition metal ion is surrounded by a certain number of ligands

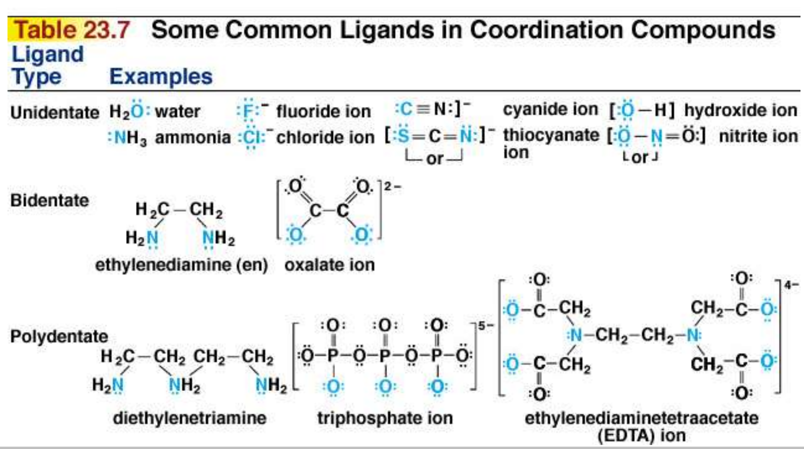
Transition metal ion : <u>Lewis acid</u>
Ligands: <u>Lewis bases</u>



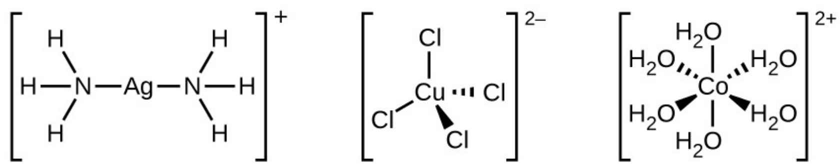
- ***<u>They primarily form coordinate covalent bonds,</u>*** a form of the Lewis acid-base interaction in which **both of the electrons in the bond are contributed by a donor (Lewis base) to an electron acceptor (Lewis acid)**
- Brackets in a formula enclose the <u>coordination sphere</u>; **species outside the brackets are not part of the coordination sphere. *<u>The coordination number of the central metal ion or atom is the number of donor atoms bonded to it</u>***

Coordination number, ligands

Ligands in Coordination Compounds

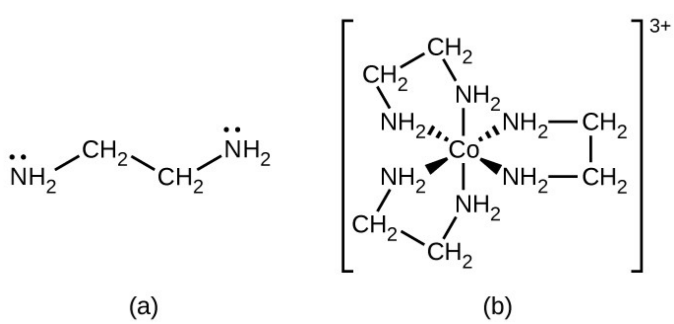


Coordination number



- The coordination number for the silver ion in $[Ag(NH_3)_2]^+$ is two
- For the copper(II) ion in $[CuCl_4]^{2-}$, the coordination number is four, whereas for the cobalt(II) ion in $[Co(H_2O)_6]^{2+}$ the coordination number is six
- Each of these ligands is <u>*monodentate, from the Greek for "one toothed," meaning that they connect with the central metal through only one atom*</u>. In this case, the number of ligands and the coordination number are equal

Coordination number



Tris(ethylenediamine)cobalt(III) chloride

Coordination number

Coordination Number	Molecular Geometry	Example
2	linear	$[Ag(NH_3)_2]^+$
3	trigonal planar	$[Cu(CN)_3]^{2-}$
4	tetrahedral(d^0 or d^{10}), low oxidation states for M	$[Ni(CO)_4]$
4	square planar (d^8)	$[NiCl_4]^{2-}$
5	trigonal bipyramidal	$[CoCl_5]^{2-}$
5	square pyramidal	$[VO(CN)_4]^{2-}$
6	octahedral	$[CoCl_6]^{3-}$
7	pentagonal bipyramid	$[ZrF_7]^{3-}$
8	square antiprism	$[ReF_8]^{2-}$
8	dodecahedron	$[Mo(CN)_8]^{4-}$
9 and above	more complicated structures	$[ReH_9]^{2-}$

Transition metal complex

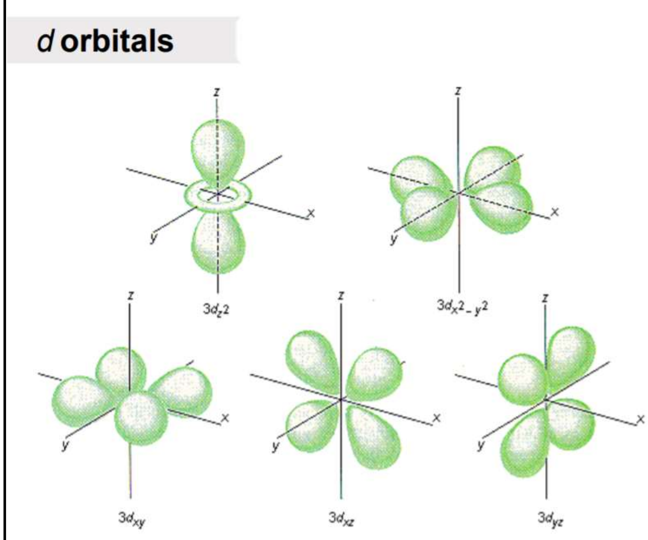
The colour can change depending on a number of factors e.g. **Metal charge and Ligand** **(How to account ?)**

Orbitals and quantum numbers

Name	Symbol	Allowed Values	Property
principal	n	positive integers (1, 2, 3,…)	orbital energy (size)
angular momentum	l	integers from 0 to n-1	orbital shape (l values of 0, 1, 2 and 3 correspond to *s*, *p*, *d* and *f* orbitals, respectively.)
magnetic	m_l	integers from $-l$ to 0 to $+l$	orbital orientation
spin	m_s	+1/2 or -1/2	direction of e^- spin

Each electron in an atom has its own unique set of four (4) quantum numbers.

Transition metal complex, d orbitals



d_{xy}: lobes lie in-between the x and the y axes.
d_{xz}: lobes lie in-between the x and the z axes.
d_{yz}: lobes lie in-between the y and the z axes.
$d_{x^2-y^2}$: lobes lie on the x and y axes.
d_{z^2}: there are two lobes on the z axes and there is a donut shape ring that lies on the xy plane around the other two lobes.

Thank you all for your attention

Information presented here were collected from various sources – textbooks, articles, manuscripts, internet and newsletters. All the researchers and authors of the above mentioned sources are greatly acknowledged.

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4th and 5th class Date : 20-09-2021

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Last class…

- Coordination complexes – introduction

In this class, laboratory component

- **Lab. : III day order : 2.10 – 3.50 pm (14 weeks, 1+8+2+2+1)**
- **Experiments:** 8 in total
- **Grading/weightage:** Each experiment carries **10 marks**
- Model practical exam and University practical exam (situation – dynamic, on campus ??)

Outline

- Aim, principle, theoretical background, the experimental details, precautions to be taken, procedure and finally calculations will be outlined and explained in class.
- Lab. Manual is already provided (GCR)
- Video of the experiment will be provided in advance (GCR)
- You need to remember/recollect the following words : Titration, equivalent weight, normal solution, end point, indicator, burette, pipette, conical flask, funnel etc …..
- Safety is important (when you are inside a lab.)

Lab. safety rules

- Applicable when in person

Outline, practical component

- In this practical component of the course you will be introduced to various **titration** methods (**volumetric analysis**)
- In **titrimetry** we add a reagent, called the **titrant**, to a solution containing another reagent, called the **titrand**, and allow them to react.
- The type of reaction provides us with a simple way to divide titrimetry into the following five categories:
- Acid-base, redox, conductometric, precipitation and complexometric titrations

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Outline

- **Acid–base titrations**, in which an acidic or basic titrant reacts with a titrand that is a base or an acid.
- **Complexometric titrations** based on metal–ligand complexation.
- **Redox titrations**, in which the titrant is an oxidizing or reducing agent.
- **Precipitation titrations**, in which the titrand and titrant form a precipitate.
- **Conductometric titration** : type of titration in which the electrolytic conductivity of the reaction mixture is continuously monitored as one reactant is added.

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Some terms (recap)

- **Titration:** A technique where a solution of known concentration is used to determine the concentration of an unknown solution. Typically, the titrant (the known solution) is added from a burette to a known quantity of the analyte (the unknown solution) until the reaction is complete.

- **Equivalent Weight (acid and base)**: The equivalent weight of an acid is that weight which yields **one mole of hydrogen ions in the reaction** employed whereas the equivalent weight of a base is that weight which reacts with one mole of hydrogen ions in the reaction.

- **Normal solution**: A solution containing **one equivalent weight of solute per litre of solution**.

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Some terms (recap)

- **Equivalence Point**: When the number of equivalents of acid (respectively base) added **is equal** to the number of equivalents of base (respectively acid) taken initially.

- **Acid-Base Indicators**: Weak organic acids or bases having different colours for their dissociated or undissociated forms

  e.g., Methyl Orange - Red (acidic solution),

  Orange – yellow (basic solution)

  pH : 3.1 – 4.6

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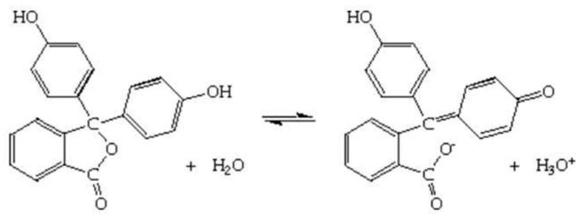
Some terms (recap)



colourless (Acid) pink (Base)

- Under acidic conditions, the equilibrium is to the left, and the concentration of the anions is too low for the pink colour to be observed in the case of phenolphthalein.
- However, under alkaline conditions, the equilibrium is to the right, and the concentration of the anion becomes sufficient for the pink colour to be observed. **pH range : 8 – 9.8**

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Equivalence point & end point

- The equivalence point is the **exact point in a titration when moles of one titrant equal the moles of the substance** being titrated.
- The endpoint is the point where the **system changes when the moles of the reacting titrant exceed the moles** of the substance being titrated.
- This can be seen as a sharp change in pH, a surge of voltage, a change in the color of the indicator, etc.
- The difference between the equivalence point and the endpoint is **an indeterminate error in all titrations (indicator error)**.

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List of experiments

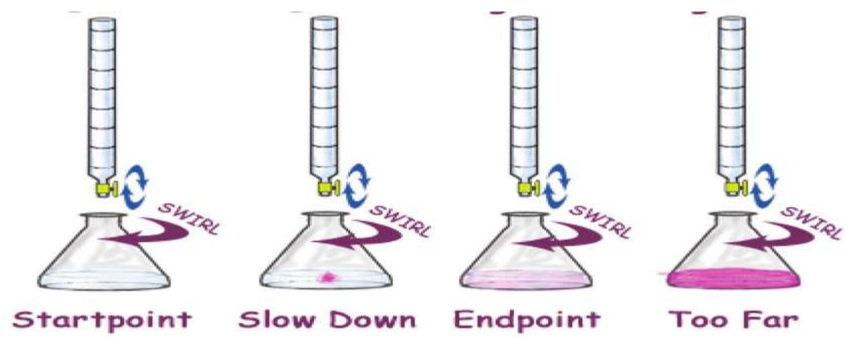
- Determination of the amount of sodium carbonate and sodium hydroxide in a mixture by titration.
- Estimation of amount of chloride content of a water sample.
- Determination of hardness (Ca^{2+}) of water using EDTA – complexometric method
- Determination of strength of an acid using pH meter.
- Determination of strength of an acid by conductometry.
- Determination of the strength of a mixture of acetic acid and hydrochloric acid by conductometry.
- Determination of ferrous ion using potassium dichromate by potentiometric titration.
- Determination of molecular weight of polymer by viscosity average method.

Acid-base titration

- A **quantitative analysis** of acids and bases; through this process, an acid or base of **known concentration** neutralizes an acid or base of **unknown concentration.**

- The titration progress can be monitored by **visual indicators**

- The reaction's **equivalence point** is the point at which the titrant has **exactly neutralized** the acid or base in the unknown analyte; if you know the volume and concentration of the titrant at the equivalence point, **you can calculate the concentration of a base or acid in the unknown solution**.



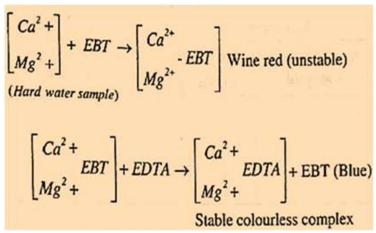
Complexometric titration

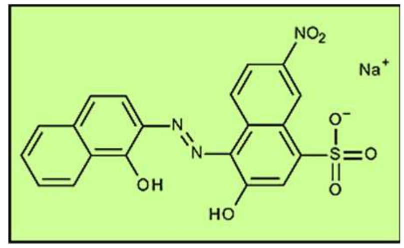
- A titration based on the formation of coordination complexes between a **metal ion and complexing agent** (or chelating agent) to form soluble complexes. ***(Hardness in water)***

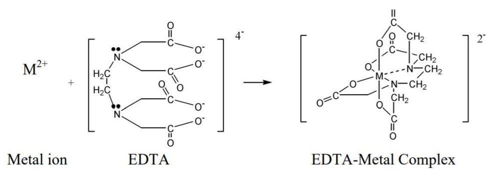
- Complex-forming reactions involving **many metal ions** can serve as a basis for accurate and convenient titrations for such metal ions. **High accuracies** and offer the possibility of determinations of metal ions at the **millimole levels**.

$$\text{Eriochrome Black-T} + Ca^{2+}/Mg^{2+} \longrightarrow \underset{\text{(Wine red)}}{\text{Eriochrome Black-T-}Ca^{2+}/Mg^{2+}}$$

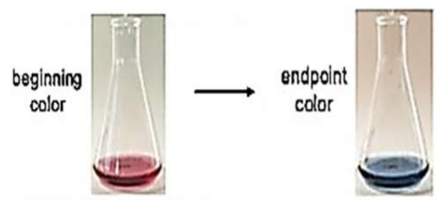
$$\underset{\text{(Wine red)}}{\text{Eriochrome Black-T-}Ca^{2+}/Mg^{2+}} + \text{EDTA} \longrightarrow \text{EDTA-}Ca^{2+}/Mg^{2+} + \underset{\text{(Steel blue)}}{\text{Eriochrome Black-T}}$$







$M^{2+} + Y^{4-} \longrightarrow MY^{2-}$



Argentometric titration (precipitation)

- A titration involving the **silver(I) ion.**

- Used to determine the **amount of chloride** present in a sample. The sample solution is titrated against a solution of silver nitrate of known concentration.

- **The indicator (potassium chromate)** is added to visualize the endpoint, demonstrating presence of silver ions, solubility product of silver chromate exceeded and it forms a **reddish-brown precipitate**. This stage is taken as evidence that all chloride ions have been consumed and only **excess silver ions have reacted with chromate ions**:

Conductometric titration

- **Electrolytic conductivity** of the reaction mixture is continuously monitored as one reactant is added.
- **The equivalence point** is the point at which the **conductivity undergoes a sudden change**. Marked increase or decrease in conductance are associated with the changing concentrations of the two **most highly conducting ions—the hydrogen and hydroxyl ions**.
- The method can be used for **titrating coloured solutions** or homogeneous suspension which cannot be used with normal indicators.

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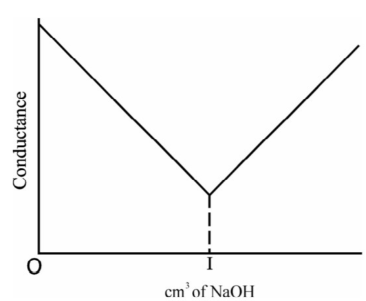
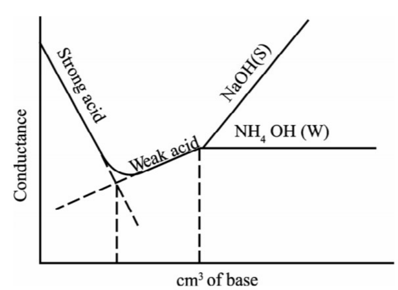
Conductometric titration, contd.





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Redox titration

- **Oxidation-reduction reaction** between the titrand and the tirant. Here the end point is detected using a potentiometer
- Potentiometric titrations involves the **measurement of the potential of a suitable indicator electrode with respect to a reference electrode** as a function of titrant volume.
- **SCE is used as the reference electrode**. Platinum metal foil, dipped in Fe^{2+} solution is used as **the indicator electrode**.

$$Cr_2O_7^{2-} + 6\,Fe^{2+} + 14H^+ \rightleftharpoons 6\,Fe^{3+} + 2Cr^{3+} + 7\,H_2O$$

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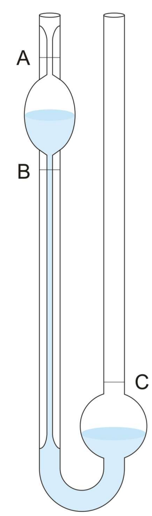
Molecular weight of a polymer

- **Viscosity** is an internal property of a fluid that offers resistance to flow.
- **Ostwald method** : viscosity of liquid is measured by **comparing the viscosity of an unknown liquid with that of liquid whose viscosity is known**.
- In this method viscosity of liquid is measured by **comparing the flow times of two liquids of equal volumes using same viscometer**.



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Work schedule

- A day before the virtual lab. class, **video of the experiment** performed by a faculty member will be shared in GCR. Lab. manual is already shared in GCR.
- **Aim, principle, methodology, procedure and calculations** will be explained in the online class
- **Practice session** – The students shall be asked to do calculations by giving model observation values for each experiment **(small lab. book and graph sheets are needed)**
- If and when you are back in campus experiments can be **carried out in the laboratories (??)**

- From next week (III order) virtual lab. sessions will be held.
- Same day the calculations and graph (if any) should be completed.
- Google form will be circulated. **Deadline - 9 pm**.
- Any clarifications needed ?
- Attendance : Kindly check everyday in student portal and if any discrepancy is seen – please alert me !!

Thank you all for your attention

Information presented here were collected from various sources – textbooks, articles, manuscripts, internet and newsletters. All the researchers and authors of the above mentioned sources are greatly acknowledged.