A Proposal for

Basic Chemistry Laboratory – II

Dr. Pratik Sen
Department of Chemistry
Indian Institute of Technology Kanpur
psen@iitk.ac.in, +91-9453105194

I. Objectives of the Virtual Lab

The objective of this virtual chemistry laboratory is to apprise the students how the real experiments were done in the laboratory to develop the theory, how a hypothesis is validated using experiment, to understand a natural phenomenon by established theory, synthesis of a drug, etc. The course will consist of experiments illustrating the principles of chemistry relevant to the study of science and engineering. All the proposed experiments are based on the topics the students learn in the theory course in chemistry in the first year.

II. List of experiments

(A Virtual Lab consists of 7-10 experiments*)

1. Rutherford scattering experiment
2. Determination of Planck constant
3. Electronic spectra of conjugated dye and test of free electron model
4. Determination of wavelength of light by diffraction method
5. Scattering experiment to understand why sky is blue
6. Estimation of entropy and free energy change of a reaction
7. Determine the pI of a glycine using potentiometric method
8. Conductometric Titration of HCl vs NaOH
9. Synthesis of Aspirin
10. Synthesis of fluorescein and its spectroscopy

(Add more as required)

The proposed experiments are not available in www.vlab.co.in. These experiments are designed based on the syllabus of BSC102 as provided in page-7 of AICTE Jan 2018, Vol-I (see below). Most of the concept in the course curriculum is covered with the proposed experiments.

II. **Undergraduate Degree courses**

Course code	BSC102				
Category	Basic Science Course				
Course title	**Chemistry-I (Theory & Lab.)** **Contents** (i) Chemistry-I (Concepts in chemistry for engineering) (ii) Chemistry Laboratory				
Scheme and Credits	**L**	**T**	**P**	**Credits**	Semester –II
	3	**1**	**3**	**5.5**	
Pre-requisites (if any)	-				

(i)Chemistry-I (Concepts in chemistry for engineering) **[L : 3; T:1; P : 0 (4 credits)]**

Detailed contents

(i) Atomic and molecular structure (12 lectures)

Schrodinger equation. Particle in a box solutions and their applications for conjugated molecules and nanoparticles. Forms of the hydrogen atom wave functions and the plots of these functions to explore their spatial variations. Molecular orbitals of diatomic molecules and plots of the multicenter orbitals. Equations for atomic and molecular orbitals. Energy level diagrams of diatomic. Pi-molecular orbitals of butadiene and benzene and aromaticity. Crystal field theory and the energy level diagrams for transition metal ions and their magnetic properties. Band structure of solids and the role of doping on band structures.

(ii) Spectroscopic techniques and applications (8 lectures)

Principles of spectroscopy and selection rules. Electronic spectroscopy. Fluorescence and its applications in medicine. Vibrational and rotational spectroscopy of diatomic molecules. Applications. Nuclear magnetic resonance and magnetic resonance imaging, surface characterisation techniques. Diffraction and scattering.

(iii) Intermolecular forces and potential energy surfaces (4 lectures)

Ionic, dipolar and van Der Waals interactions. Equations of state of real gases and critical phenomena. Potential energy surfaces of H_3, H_2F and HCN and trajectories on these surfaces.

(iv) Use of free energy in chemical equilibria (6 lectures)

Thermodynamic functions: energy, entropy and free energy. Estimations of entropy and free energies. Free energy and emf. Cell potentials, the Nernst equation and applications. Acid base, oxidation reduction and solubility equilibria. Water chemistry. Corrosion. Use of free energy considerations in metallurgy through Ellingham diagrams.

(v) Periodic properties (4 Lectures)

Effective nuclear charge, penetration of orbitals, variations of s, p, d and f orbital energies of atoms in the periodic table, electronic configurations, atomic and ionic sizes, ionization energies, electron affinity and electronegativity, polarizability, oxidation states, coordination numbers and geometries, hard soft acids and bases, molecular geometries

(vi) Stereochemistry (4 lectures)

Representations of 3 dimensional structures, structural isomers and stereoisomers, configurations and symmetry and chirality, enantiomers, diastereomers, optical activity, absolute configurations and conformational analysis. Isomerism in transitional metal compounds

(vii) Organic reactions and synthesis of a drug molecule (4 lectures)

Introduction to reactions involving substitution, addition, elimination, oxidation, reduction, cyclization and ring openings. Synthesis of a commonly used drug molecule.

*Alternatively, 3-4 additional experiments (minimum) may be developed to augment existing labs (www.vlab.co.in).

Note: Please list all related experiments available on the web (vlab.co.in) and compare your proposed experiments with them. Please justify why the proposed experiments are needed and exactly what gaps they fill.

III. **Target group of users**

- UG (1st Year/ 2nd Year) [highest priority for development]

This is a second semester course and the students from all branches will take this course.

IV. **Mapping of proposed lab with AICTE courses as per attached list of potential labs**

- Course name and Code

BSC102, Chemistry-I

V. **Mapping of proposed lab with universities** (minimum 3 universities)

- Name of University; Course code; Course name

Calcutta University, CEMA-CC-1-1-TH, BSc., Chemistry-2

The University of Burdwan, CC-3, UG, Structure of Atom

JC Bose University of Science and Technology, YMCA, Faridabad, UG, BSC-105 (LAB), Chemistry Theory and Lab

Lovely Professional University, CHE113, UG, Basic Inorganic Chemistry

Neheru Gramvarti University, Prayagraj, BOC-101, BSc., Inorganic Chemistry; BOC-103, BSc., Physical Chemistry

NIT Hamirpur, CY613, UG, Physical Chemistry-I

BRA Bihar University, Muzaffarpur, Chemistry Paper-I, Chemistry Paper-II, BSc.

VI. **Expected timelines**

Presentation of proposal to domain experts' committee – 31st March 2022

Demo of First 3 Expts and Review – 30th June 2022

Demo of 5-6 Expts and review – 31st August 2022

Demo of 7-10 Expts and review – 31st October 2022

Final demo of 7-10 Expts – 15th November 2022

Hosting of lab (7-10 Expts) – 30th November 2022

Note 1: The LDC will coordinate the reviews and hosting

Note 2: The lab is supposed to be developed and hosted within 6 - 9 months from the date of approval

VII. **Budget** (Max. Rs 2 Lakhs per experiment with a ceiling of Rs 20 Lakhs per Lab)

Table I. Budget for Basic Science Course, BSC102

S. No.	Equipment/Activity	Budget # (In Rupees)
1	Laptop / Machine	6,65,000
2	Manpower	3,94,200
3	Consumables	6,50,000
4	Contingency	1,00,000
5	Honorarium for Lab Developer (Rs 20k per experiment; Ceiling of Rs 2 Lakhs per lab)	1,00,000
6	Miscellaneous	60,000
TOTAL		19,69,200

To be released based on the recommendation of the review committee
Note: Institute overheads not to be included in the budget

VIII. **Justification of the budget requirements**

(a) Details of Laptop/Machine

One laptop, Rs. 65,000/-
Laser, Rs. 5,00,000/-
Analytical Balance, Rs. 1,00,000/-

(b) Details of Manpower (number, cost per man-months etc.)

a. Total man-months required

18

b. No. of project staff, cost per man-months

Project Scientist: One (1), Rs. 35,000/- per month
Project Attendant: One (1), Rs. 8,800/- per month

c. Honoraria for other staff associated with the project

Honoraria for chemistry laboratory staffs Rs. 10,000/- per experiments.

(c) Details of Consumables

Varieties of consumables are needed to optimize and develop the proposed experiments. For example, chemicals, solvent, light source, optical components, etc.

(d) Details of Miscellaneous cost

a. Internal Review (Optional, Rs 1000 per experiment)

Internal review by faculty members will be done for each experiment. For a total 10 experiments, the cost will be Rs. 10,000/-

b. Field Trials

Not applicable

c. Others

Video recording of laboratory experiments for giving the students an in-laboratory experience. The cost is Rs. 5,000/- per hour. For 10 experiments of approximately 1 hr each, the total cost will be Rs. 50,000/-.

IX. Student Feedback and Learning

- How will you collect feedback and use them?

The feedback will be collected in terms of google form for each experiments. After receiving a few of them, or periodically, the inputs will be analyzed by the PI. If needed, a modification of thee virtual lab will be done and will be updated in the system.

- What is the actual learning component provided by the Virtual Lab?

The take home learning of the proposed virtual lab are as follows:

Experiment 1: How Rutherford determined the size of nuclei and concluded that most part of the atom is empty.
Experiment 2: Planck constant is a very small number, but not zero.
Experiment 3: The validity of quantum mechanical particle in a box model.
Experiment 4: How to determine the wavelength of a light.
Experiment 5: Why the sky is blue on a sunny day, yet red or orange at sunrise and sunset.
Experiment 6: How to estimate free energy change of a reaction.
Experiment 7: How to determine the isoelectric point.
Experiment 8: How to measure conductance and how to follow a reaction using conductometry.
Experiment 9: How to synthesize a drug (Aspirin)
Experiment 10: About the property of fluorescence.

- After the Virtual Lab experience, would the student be able to perform the experiment in the real lab?

Along with the virtual lab, a short video of performing the experiment in real laboratory will be provided. This will give the students an idea about the real life in-hand experience virtually. Care will be taken to introduce each equipment.

1. Rutherford scattering experiment

Objective:
To simulate Rutherford backscattering experiment and find the size of nuclei from scattering probability.

Theory:
Rutherford's gold foil experiment showed that the atom is mostly empty space with a tiny, dense, positively-charged nucleus. Based on these results, Rutherford proposed the nuclear model of the atom.

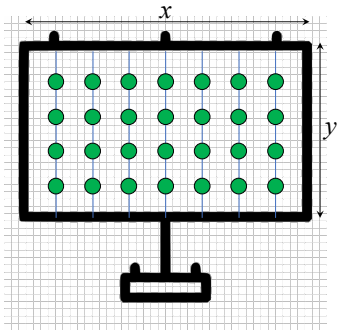


Figure 1. Modelling Rutherford backscattering experiment with Ping-Pong ball.

Ernest Rutherford got the idea that the structure of atoms could be probed by observing the scattering of alpha particles. Alpha particles, as Rutherford himself had demonstrated, are the positively charged discharges of radioactive substances. They are the bare helium nuclei. According to the raisin pudding model, an alpha particle traversing a thin gold film should experience many small angle deflections as it passes close to or through the positive spheres of the gold atoms. This prediction turned out to be correct for very small angles of scattering. But in experiments initiated at Rutherford's direction, Geiger and Marsden (1909) found that 1 in 8000 alpha particles passing through a thin film of gold was scattered through more than 90°. It was as though bullets fired at a bale of cotton could occasionally ricochet backward. Such an observation might lead one to suspect rocks in the cotton.

At this point Rutherford (1911) advanced the hypothesis that the positive charge and most of the mass of an atom is concentrated in a "nucleus" with dimensions of the order of 10^{-12} cm (10,000 times smaller than the atom as a whole) with the electrons in some sort of configuration around it.

In this experiment, we will model Rutherford's experiment with Ping-Pong balls and will estimate the size of the nucleus (a ping-pong ball). A model of monolayer gold atom will be prepared as shown in Fig. 1. As in the case of gold, most of the part of the monolayer are occupied by electron (free space in the model). Several (300-400) ping-pong balls will be thrown to the model and the number of back scattered ball will be counted. From this the probability of backscattering will be calculated as,

$$P = \frac{\#\ ball\ backscattered}{total\ \#\ balls} = \frac{Total\ area\ of\ nuclei}{Total\ area\ of\ atoms} = \frac{Total\ area\ of\ nuclei}{xy} \qquad (1)$$

For this experiment the probability of backscattering will be measured and from equation (1) the area, thus the diameter of ping-pong ball (nucleus) will be estimated.

2. Determination of Planck constant

Objective:
To apprise that the value of the Planck constant is very small, but not zero.

Theory:
An LED is a semiconductor light source. In the unbiased condition a potential barrier is developed across the *p*-*n* junction of the LED **(Fig 1)**. When we connect the LED to an external voltage in the forward biased condition, holes from the *p* type and electrons from the *n* type region start to enter the junction to enable the current flow and as a result the height of potential barrier across the p-n junction is reduced. At a particular voltage in this forward biased condition, the height of the potential barrier becomes so low that the current flow increases rapidly and the LED starts glowing as the excited electrons (the electrons which are crossing the junction) comes to the ground state (valence band). This particular voltage is called the knee voltage or the threshold voltage. Once the knee voltage is reached, the current may increase but the voltage does not change.

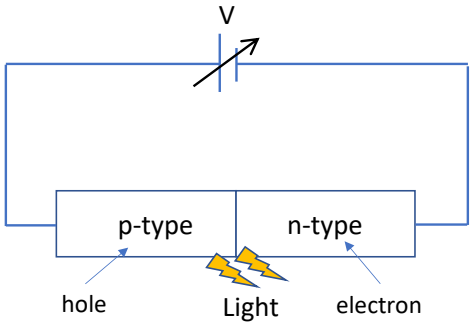


Figure 1. Working Principle of LED

The light energy emitted during forward biasing is given as

$$E = \frac{hc}{\lambda} \qquad (1)$$

where, c is the velocity of light, h is the Planck's constant and λ is the wavelength of the emitted light. If V is the forward voltage applied across the LED when it begins to emit light (the knee voltage), the energy given to electrons crossing the junction is:

$$E = eV \qquad (2)$$

From equation (1) & (2), we get

$$V = \frac{hc}{e} \times \left(\frac{1}{\lambda}\right) \qquad (3)$$

The knee voltage V can be measured for LEDs with different values of λ (wavelength of emitted light). Now from equation (4), we see that the slopes of a graph of V vs $\frac{1}{\lambda}$ is $\frac{hc}{e}$.

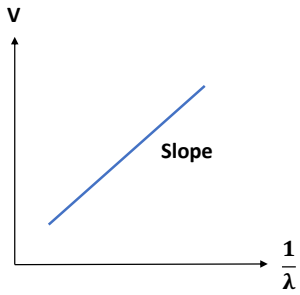


Figure 2. Plot of knee voltage as a function of inverse wavelength of LED.

$$h = slope \times \left(\frac{e}{c}\right) \qquad (4)$$

Therefore, Planck constant can be determined by using equation (4).

3. Electronic spectra of conjugated dye and test of free electron model

Objective:
Students will learn the measurement of absorption spectrum and will interpret the absorption spectrum conjugated molecules using the free-electron model.

Theory:
Absorption in the visible region of the spectrum correspond to transitions from the ground electronic state of a molecule to an excited electronic state. For π-conjugated organic molecule, the transition is typically π-π* in nature, and they appeared to be colored.

Some of these compounds that will be investigated are –

1,4 – diphenyl – 1,3 – butadiene
1,6 – diphenyl – 1,3,5 – hexatriene
1,8 – diphenyl – 1,3,5,7 - octatetraene

We shall present here the simple free-electron model first proposed by Kuhn for successfully determining the energy of absorption for molecules like a conjugated dye. We shall assume that the potential energy is constant along the chain and that it rises sharply to infinity at the ends; i.e., the π electron system is replaced by the free electrons moving in a one- dimensional box of length L. The quantum mechanical solution for the energy levels of this model is

$$E_n = \frac{n^2h^2}{8mL^2} \; ; n = 1,2,3 \ldots \qquad (1)$$

where m is the mass of an electron, n is quantum number and h is the Planck constant.

Since the Pauli exclusion principle limits the number of electrons in any given energy level to two (these two have opposite spins: +½, -½) the ground state of a molecule with N π-electrons will have the N/2 lowest levels filled and all higher levels empty. When the molecule absorbs light, this is associated with one electron jump from the highest filled level (n_1 = N/2) to the lowest empty level (n_2 = N/2 + 1). The energy change for the transition is

$$\Delta E = E_{N/2+1} - E_{N/2} = \frac{h^2}{8mL^2}\left[\left(\frac{N}{2}+1\right)^2 - \left(\frac{N}{2}\right)^2\right] = \frac{(N+1)h^2}{8mL^2} \qquad (2)$$

Since ΔE = $h\nu = \frac{hc}{\lambda}$, where c is the speed of light and λ is the wavelength,

$$\lambda = \frac{8mL^2c}{(N+1)h} \qquad (3)$$

From the above equation, wavelength of the transition at the absorption maxima can be determined for the compounds mentioned above. For each compound N is determined by counting the number of π electrons between the phenyl rings. The lowest energy transition occurs from the highest occupied energy level to the lowest unoccupied energy level. For example, 1,4-diphenyl-1,3-butadiene contains 4 π electrons between the phenyl rings. Thus, $N = 4$. In this series of diphenyl compounds, the length of the box is taken to be the distance between the phenyl rings.

4. Determination of wavelength of light by diffraction method

Objective:

Students will learn how to determine the wavelength of a light using diffraction grating with the help of the law of diffraction.

Theory:

The diffraction of classical waves refers to the phenomenon wherein the waves encounter an obstacle that fragments the wave into components that interfere with one another. Interference simply means that the wavefronts add together to make a new wave which can be significantly different than the original wave. Here we will be using the diffraction grating that gives rise to the diffraction phenomenon. It consists of a transparent material into which a very large number of uniformly spaced wires have been embedded (Fig. 1). As the light impinges on the grating, the light waves that fall between the wires propagate straight on through. At certain points in the forward direction the light passing through the spaces (or slits) in between the wires will be in phase and will constructively interfere. Whenever the difference in path length between the light passing through different slits is an integral number of wavelengths of the incident light, the light from each of these slits will be in phase, and it will form an image at the specified location. Mathematically, the relation is simple:

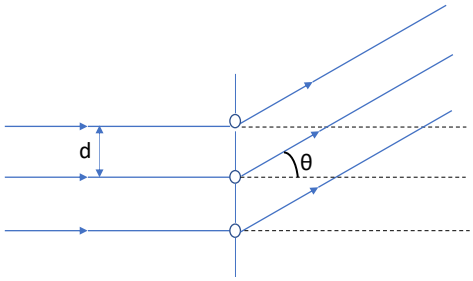


Figure 1. Geometry determining the conditions for diffraction from a multi-wire grating.

$$m\lambda = d \sin\theta \qquad (1)$$

In the above equation, d is the distance between adjacent slits (which is the same is the distance between adjacent wires) (Fig. 1), θ is the angle the re-created image makes with the normal to the grating surface, λ is the wavelength of the light, and m = 0, 1, 2, . . . is an integer.

By shining a light beam into a grating whose spacing (d) is known, and measuring the angle θ where the light is imaged, one can measure the wavelength λ. Consider Fig. 2, which shows the set-up for a diffraction grating experiment. If a monochromatic light source shines on the grating, images of the light will appear at several angles—θ_1, θ_2, θ_3 and so on. The value of θ_m is given by the grating equation shown above, so that

$$\theta_m = \sin^{-1}\left(\frac{m\lambda}{d}\right) \qquad (2)$$

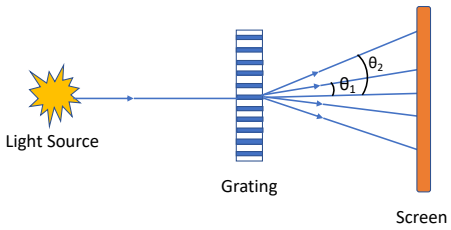


Figure 2. Experimental set-up for measuring wavelengths with a diffraction grating

The image created at θ_m is called the m^{th} order image. The 0^{th} order image is the light that shines straight through. Here we will be looking at the first and second order diffraction images of a laser and measuring its wavelength.

5. Scattering experiment to understand why sky is blue

Objective:
Acquainting the students the phenomenon of scattering and why the sky is blue on a sunny day, yet red or orange at sunrise and sunset.

Theory:
The colour of the sky changes during sunrise and sunset time from the daytime because of the different extend of scattering of the sunlight by the particles present in the atmosphere. The sunlight has to cross the atmosphere before it reaches our eyes. If we think that the atmosphere acts like a coating covering of the Earth, sunlight at noon passes through the thinnest part of the coating as the sun is just above us i.e. closest to the Earth. So in this case the scattering is less as there is least number of particles in the path. During sunrise and sunset, light has to take a sideways path to the same point, through a lot more "coating", which means there are a lot more particles that can scatter light more. While multiple types of scattering occur in the Earth's atmosphere, Rayleigh scattering is primarily responsible for this.

In this experiment a transparent container is filled partially with water. Now if we turn on the flashlight and hold it flat against the side of the container, we won't be able to see the beam of the flashlight. This is much like how sunlight travels through space. Now we add some small amount of milk and stir the mixture. Now, if we shine the flashlight again from the previous position, we can see the beam of light in the water. If we now examine the container from all sides, the flashlight beam looks slightly blue from the side of the container, while the end of the flashlight appears slightly yellow. If we add more milk into the water, the beam appears even bluer from the side of the container, while the path of the beam farthest from the container changes from yellow to orange. The beam also spread out as it crosses the container. The blue end is like the sky at noon on a clear day. The orange end is like the sky near sunrise or sunset.

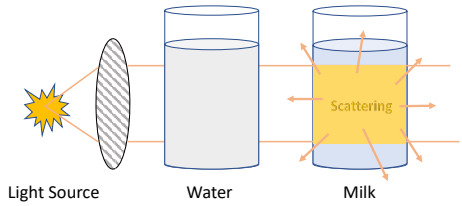


Figure 1. Illustration of scattering through the milk/water solution

Light travels in a straight line until it encounters particles where it gets deflected or scattered. In pure air or water, you can't see a beam of light and it travels along a straight path. When there are particles in the air or water, light is scattered by the edges of the particles. Milk is a colloid that contains tiny particles of fat and protein. When mixed with water, the particles scatter light much as dust scatters light in the atmosphere. Light is scattered differently, depending on its colour or wavelength, as well as depends on the size of the particle. In visible region of the electromagnetic spectrum, violet-blue light is scattered the most, while the orange and red light is scattered the least. Looking at the daytime sky is like viewing a flashlight beam from the side where we see the scattered blue light. Looking at sunrise or sunset is just like looking the beam across the container where we see the light that isn't scattered, which is orange and red. As we increase the amount of milk, the number of colloidal particles in the water will be increased and the beam of the flashlight is more strongly scattered, and the blue and orange part will become more intense.

6. Estimation of entropy and free energy change of a reaction

Objective:
To let the students understand how to measure the enthalpy, entropy and Gibbs free energy change.

Theory:
Borax is sparingly soluble in water. The equilibrium expression for the process that gives two sodium ions, one borate ion, $B_4O_5(OH)_4^{2-}$, and ten water molecules is

$$Na_2B_4O_5(OH)_4\ 10H_2O\ (s) \rightleftharpoons 2Na^+(aq) + B_4O_5(OH)_4^{2-}\ (aq) + 10\ H_2O\ (l) \quad (1)$$

The reaction can be written in simplified form as:

$$\text{Borax}\ (s) \rightleftharpoons 2Na^+(aq) + \text{Borate}\ (aq) + 10\ H_2O\ (l) \quad (2)$$

Since liquid water and solid borax are not included in the K_{sp} expression, the solubility product expression associated with this reaction is:

$$K_{sp} = [Na^+]^2\ [\text{Borate}] \quad (3)$$

The concentration of the borate ion in equilibrium will be determined by titration with standardized HCl according to the equation:

$$B_4O_5(OH)_4^{2-}(aq) + 2HCl\ (aq) + 3\ H_2O\ (l) = 4H_3BO_3\ (aq) + 2Cl^-(aq) \quad (4)$$

According to equation (4), two moles of HCl are required for 1 mol of borate. Thus,

$$[B_4O_5(OH)_4]^{2-} = \frac{Moles\ of\ HCl\ required\ for\ titration}{2 \times Volume\ of\ solution\ required} \quad (5)$$

Also from the stoichiometric relationship in equation (1): 1 mole borate ≡ 2 mole Na^+. Thus,

$$[Na^+] = \frac{1}{2}\ [B_4O_5(OH)_4^{2-}] \quad (6)$$

K_{sp} of borax can be calculated from the values of $[B_4O_5(OH)_4^{2-}]$ and $[Na^+]$. The K_{sp} for borax will be evaluated at room temperature (T_1) and at about 278 K (T_2). K_{sp} values at two temperatures allows the evaluation of the enthalpy change using Equation (7).

$$\ln\frac{K_{sp1}}{K_{sp2}} = \frac{\Delta H}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right) \quad (7)$$

Knowing the solubility product constant at two different temperatures also allows the evaluation of the Gibbs free energy change (ΔG°) at each of the two temperatures using Equation 8.

$$\Delta G^o = -\ RT\ \ln(K_{sp}) \quad (8)$$

Remember that ΔH and ΔS are not supposed to change with temperature. On the other hand, ΔG usually does change appreciably with temperature. Once ΔH^o (same as ΔH) and ΔG^o values are known for each temperature, the values of the entropy change, ΔS^o, at each temperature can be evaluated using equation (9).

$$\Delta G^o = \Delta H^o - T\ \Delta S^o \quad (9)$$

7. Determine the pI of a glycine using potentiometric method

Objective:

In this experiment the students will learn how to determine the isoelectric point of an amino acid by titrating it with a standard base.

Theory:

Proteins and amino acids contain both acidic (–COOH) and basic ($–NH_2$) groups in their structures and are amphoteric in nature. The net molecular charges of such molecules can vary depending upon the pH of the medium. Hence if we apply an electric field across the solution, the molecules will move towards either cathode or anode depending upon the nature of the charge. The isoelectric point (pI) is the pH at which a molecule carries no net charge and hence will not show any movement in the electric field. When pH < pI, molecules carry a net positive charge and when pH > pI, they carry a net negative charge.

For an amino acid having only one $–NH_2$ and one –COOH group, the calculation of pI can be very simple if the pKa values are known. Glycine is the simplest amino acid containing one $–NH_2$ and one –COOH group. It can exist in three ionic forms: H_3N^+-CH_2-COOH (at pH = 1), H_3N^+-CH_2-COO^- (at pH = 6) and H_2N-CH_2-COO^- (at pH = 11). The two pKa values arise from the equilibrium given in Fig. 1.

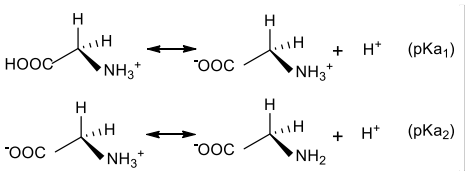


Figure 1. Protonation and de-protonation of glycine

pI can be written as

$$pI = \frac{pKa_1 + pKa_2}{2} \qquad (1)$$

The determination of isoelectric point (equivalence point) of titrations based on potential measurements is called potentiometric titration. The equivalence point is indicated by a large change in the potential. A good potentiometric titration requires a suitable working electrode and a standard reference electrode. This is where pH meter can be used. Let us consider the potentiometric titration of glycine vs NaOH solution. With the gradual addition of NaOH, the change in pH will be similar to the curve given in Fig. 2.

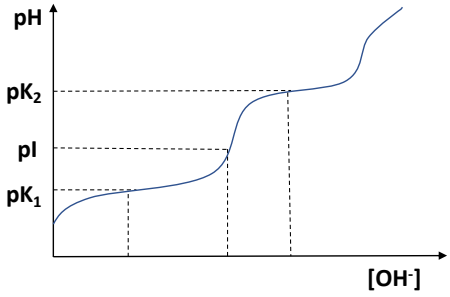


Figure 2. pH titration of glycine with NaOH

As we can see in the titration curve, it has two dissociation steps corresponding to loss of H^+ from the acidic carboxyl group at low pH followed by loss of H^+ from the more basic amino group at high pH. The pKa value for each dissociable group of an amino acid can be determined from such a titration curve by extrapolating the midpoint of each buffering region (the plateau) in the titration curve. The diagram also shows that there is a point in the curve where the amino acid behaves as a neutral salt. At this pH, the amino acid is predominantly a zwitterion with a net charge of zero. This point of the titration curve is the isoelectric point (pI) and can be approximated as halfway between the two points of strongest buffering capacity (the two pKa values).

8. Conductometric Titration of HCl vs NaOH

Objective:

To let the students understand how to measure conductance and how to follow a reaction using conductometry.

Theory:

An electrolytic solution is capable to conduct current due to the presence of ions that act as a charge carrier in the solution. For such a system it is more convenient to describe the current flowing capacity by the conductance, *L*, (in mhos or ohms^{-1}), rather than by the resistance, *R*. Nevertheless, they are related as

$$L = \frac{1}{R} = \kappa \frac{A}{l} \qquad (1)$$

The resistance (R) depends upon the nature and geometry of the conductor and κ is the specific conductance, i.e., the conductance of a tube of material 1 cm long having a cross section of 1 cm2. The unit of κ is mho cm^{-1}.

The equivalent conductance (Λ: cm^2 Ohm^{-1} mole^{-1}) is defined as the conductance of a solution containing 1 gm-equivalent of electrolyte such that the entire solution is placed between two electrodes 1 cm apart. The specific conductance of an electrolyte solution is related to equivalent conductance by

$$\Lambda = \frac{\kappa}{c} \qquad (2)$$

Strong electrolytes, such as HCl, dissociate fully into ions when dissolved in water and the conductance of this solution can be written as the summation of the individual ionic conductance

$$\Lambda_{HCl} = \lambda_{H^+} + \lambda_{Cl^-} \qquad (3)$$

The principle of conductometric titration is based on the fact that during the titration, one of the ions is replaced by the other and invariably these two ions differ in the ionic conductivity with the result that conductivity of the solution varies during the course of titration. The equivalence point may be located graphically by plotting the change in conductance as a function of the volume of titrant added.

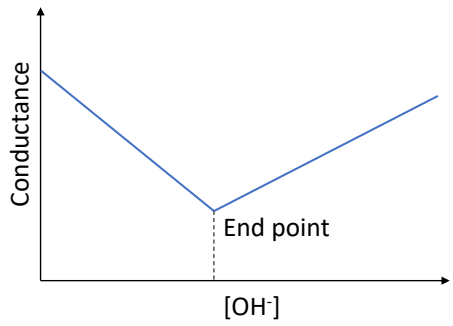


Figure 1. Conductometric titration of HCl with NaOH

Now consider the case where HCl is being titrated with a strong base NaOH as titrant. Before NaOH is added, the conductance is high due to the presence of highly mobile hydrogen ions, as given by equation (3). When the base is added, the conductance falls due to the replacement of hydrogen ions by the added Na^+ cation which has very less ionic conductance than H^+ as H^+ ions react with OH^- ions to form undissociated water as follows:

$$H^+(aq) + Cl^-(aq) + Na^+(aq) + OH^-(aq) \rightarrow Na^+(aq) + Cl^-(aq) + H_2O(l)$$

This decrease in the conductance continues till the equivalence point (Fig. 1). At the equivalence point, the solution contains only NaCl. After the equivalence point, the conductance increases due to the large conductivity of OH^- ions.

The strength of the acid can now be calculated via the formula: $S_2 = (V_1S_1)/V_2$, where S_2 is the strength of the acid, V_1 is the volume of NaOH added at the equivalence point, S_1 is the strength of the NaOH (already known) and V_2 is the volume of HCl (V_2) (also known).

9. Synthesis of Aspirin

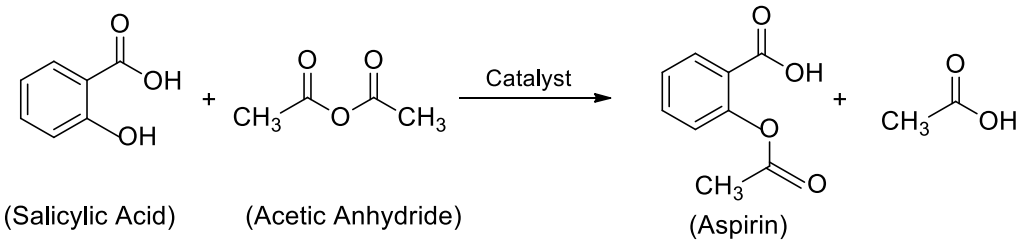
Objective:

Students will learn how to synthesize the famous drug aspirin or acetylsalicylic acid, that is used to reduce pain, fever or inflammation.

Theory:

The discovery of aspirin was inspired by Felix Hoffman's attempt to find a drug to ease his father's arthritis without causing the severe stomach irritation associated with the standard anti-artharitis drug of the time, sodium salicylate. The name aspirin is believed to be derived from the "A" of acetyl and the "spir" of spiraea, the botanical name of the meadowsweet plant from which salicylic acid was first chemically isolated. Aspirin is one of the oldest and most useful drugs known. Salicylates are antipyretics; that is, they lower the body temperature of one who has a fever but have little effect if the temperature is normal. Salicylates are also mild analgesics, which relieve certain types of pain (such as headache, neuralgia, and rheumatism). The best known form of aspirin is Alka Seltzer, which also contains citric acid and sodium bicarbonate. Aspirin is not very soluble in water; its solubility is only about 0.25 g/100 ml. The bicarbonate reacts with aspirin to form its sodium salt, thereby making it water soluble and quicker in action. The bicarbonate reacts with citric acid to form carbon dioxide and the citric acid makes the taste of aspirin.

Aspirin can simply be prepared in the laboratory by acetylation of salicylic acid. In this preparation, we will heat a mixture of salicylic acid and acetic anhydride with a little concentrated sulfuric as catalyst. The formed acetylsalicylic acid can be redissolved in ethanol and then recrystallized further from water. Acetylsalicylic acid crystallizes as needle-like crystals with a melting point of 135 °C. It is odorless, but in moist air it gradually hydrolyzes into acetic and salicylic acids.



(Salicylic Acid) (Acetic Anhydride) (Aspirin)

10. Synthesis of fluorescein and its spectroscopy

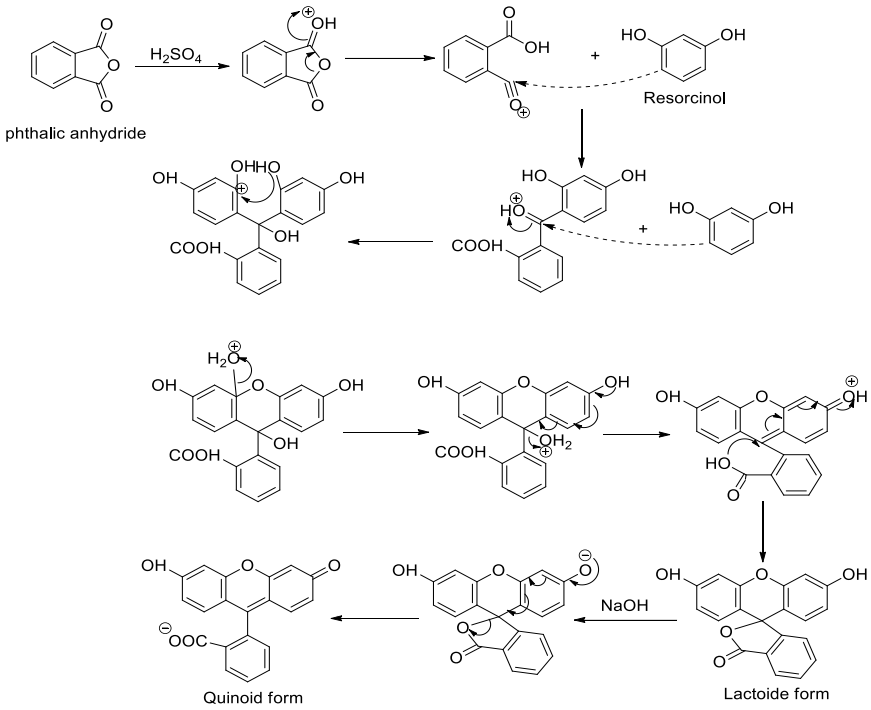
Objective:

To apprise students the synthesis of famous fluorophore fluorescein and its fluorescence property.

Theory:

Fluorescein is a brown-red to yellow powder, which is poorly soluble in water. In sodium or potassium hydroxide solution or in ethanol, it readily dissolves giving an intense greenish yellow fluorescence. Two forms of the compound are known, the more stable quinoid dark-red acid free form and a less stable lactoide form, which is yellow in color. On acidification of the fluorescent solution, the fluorescence decreases as only the anion carries the characteristic fluorescence. The dye absorbs light in the blue range of the visible spectrum, with absorption peaking at 490 nm (blue). An additional peak is also observed at 460 nm. It emits light at 530 nm (yellow). The fluorescence and absorbance of fluorescein is quite pH sensitive.

Fluorescein can be synthesized through the reaction between phthalic anhydride and resorcinol through the following pathway in the presence of acid as a catalyst.



Fluorescein angiography, also known as "the yellow dye test" is a way of assessing various disease states in the retina and choroid of the human eye. Actually, the sodium salt of fluorescein is used for angiography. A small amount of sodium fluorescein dye is injected into a vein in the patient's arm (normal adult dosage is 500 mg). A special camera is used to view the retina of the eye. The blue-colored light coming from the camera causes the sodium fluorescein dye to glow in a yellow-green color. As the sequence begins, the image is black because no sodium fluorescein is present in the vessels. A second or so after reaching the choroid, the dye begins to fill the retinal vessels. The arteries become visible first. The dye then travels across the network of fine capillaries, where nutrients and oxygen are transferred to tissue. The dye continues its journey through the retina, filling the veins and exiting the eye. Photographs are usually taken at intervals up to about 10 minutes after the injection of the dye. An ophthalmologist examines the way the fluorescein dye travels through the vessels during the transit phase and the way in which the dye pools or stains tissues in the later phases as a part of the diagnostic process for determining causes of decreased vision.

ANNEXURE-I

Important information for the development of Virtual Labs

(A Virtual Lab consists of 7-10 experiments)

X. **Link to some sample virtual labs**

https://python-iitk.vlabs.ac.in/ https://cs-iitd.vlabs.ac.in/ https://plchla-coep.vlabs.ac.in/

XI. **Technology Used**

- For Web interface (should be Free and Open-Source Software)
- For back-end (should be Free and Open-Source Software)

XII. **Required Components for virtual experiments**

- Step-by-step procedure
- Online manual
- Pre-test
- Simulator
- Post-test
- Related resources
- Additional help

All the above requirements will be fulfilled on sanction of the project.