#### UG - I

## Titratimetric Determination of Acid Content in Freshly prepared Orange Juice/ Lemon Juice

The project work is designed to impart knowledge and expertise with the natural products (lemon juice) or commercially available beverages and carry out their titrations for quantitative estimation (i.e. vitamin C in lemon juice or orange juice or commercially available fruit juice). It is related to the syllabus of CHEM01C1: Lab (Acid-Base Titration).

#### UG - II

## Titrimetric Determination of Vitamin-C in a commercially available tablet

This project is designated to train the students to determine the amount of vitamin C in commercial tablet by redox titration. It is related to the syllabus of CHEM03C5: Lab (Iodo/Iodometric Titrations).

## Synthesis of Dibenzylidene acetone as a constituent of Sunscreens through Aldol Condensation

This project is designated to train the students to prepare industrially relevant molecules. During the preparation they are going to learn new purification techniques of organic molecules. It is related to the syllabus of CHEM03C6: Lab (Aldol condensation).

### PG-I

Numerical Solution of Langevin equation and verification of kinetic theory of gas / Stochastic Study of the temperature dependent Electron Transfer Kinetics in the Reaction Centers of Purple Photosynthetic Bacterium

The project is designed for realizing applications of numerical simulation methods (so: of deferential equns) in the content of chemical sciences. It is related to the syllabus of CHEM0892 (Interpolation, numerical integration, numerical solution of differential equations).

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BeF<sub>2</sub>, CO<sub>2</sub>, (idea of s-p mixing and orbital interaction to be given). Formal charge, Valence shell electron pair repulsion theory (VSEPR), shapes of simple molecules and ions containing lone pairs and bond pairs of electrons, multiple bonding ( $\sigma$  and  $\pi$  bond approach) and bond lengths.

Covalent character in ionic compounds, polarizing power and polarizability. Fajan's rule and consequences of polarization.

Ionic character in covalent compounds: Bond moment and dipole moment. Percentage ionic character from dipole moment and electronegativity difference.

(iii) Metallic Bond: Qualitative idea of valence bond and band theories. Semiconductors and insulators, defects in solids.

(iv) Weak Chemical Forces: van der Waals forces, ion-dipole forces, dipole-dipole interactions, induced dipole interactions, Instantaneous dipole-induced dipole interactions. Repulsive forces, Hydrogen bonding (theories of hydrogen bonding, valence bond treatment) Effects of chemical force, melting and boiling points.

(20 Lectures)

#### Oxidation-Reduction:

Elementary idea on standard redox potentials with sign convention, Nernst equation. Influence of complex formation, precipitation and change of pH on redox potentials, formal potential. Feasibility of a redox titration, redox potential at the equivalence point, redox indicators, redox potential diagram (Latimer and Frost) of common elements and their applications. Disproportionation and comproportionation reactions (typical examples).

### Reference Books:

- Lee, J.D. Concise Inorganic Chemistry ELBS, 1991.
- Douglas, B.E. and McDaniel, D.H. Concepts & Models of Inorganic Chemistry Oxford, 1970
- Atkins, P.W. & Paula, J. Physical Chemistry, 10th Ed., Oxford University Press, 2014.
- Day, M.C. and Selbin, J. Theoretical Inorganic Chemistry, ACS Publications, 1962.
- Rodger, G.E. Inorganic and Solid State Chemistry, Cengage Learning India Edition, 2002.

### CHEMISTRY PRACTICAL- C1 LAB:

(Credits: Practicals-02, 60 Lectures, Full marks: 30)

Elementary idea of redox titration using KMnO<sub>4</sub> and K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> (theory)

- (A) Titrimetric Analysis
- (i) Calibration and use of apparatus
- (ii) Preparation of solutions of different Molarity/Normality of titrants
- (B) Acid-Base Titrations
- (i) Estimation of carbonate and hydroxide present together in mixture.

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#### Reference Books:

- Lee, J.D. Concise Inorganic Chemistry, ELBS, 1991.
- Douglas, B.E; Mc Daniel, D.H. & Alexander, J.J. Concepts & Models of Inorganic Chemistry 3rd Ed., John Wiley Sons, N.Y. 1994.
- Greenwood, N.N. & Earnshaw. Chemistry of the Elements, Butterworth-Heinemann. 1997.
- Cotton, F.A. & Wilkinson, G. Advanced Inorganic Chemistry, Wiley, VCH, 1999.
- Rodger, G.E. Inorganic and Solid State Chemistry, Cengage Learning India Edition, 2002.
- Miessler, G. L. & Donald, A. Tarr. Inorganic Chemistry 4th Ed., Pearson, 2010.
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- Atkin, P. Shriver & Atkins' Inorganic Chemistry 5th Ed. Oxford University Press (2010).

### CHEMISTRY PRACTICAL - C5 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

## (A) Iodo / Iodimetric Titrations

Principles involved in iodometric titration

- (i) Estimation of Cu(II) and K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> (Iodimetrically).
- (ii) Estimation of available chlorine in bleaching powder iodometrically.

## (B) Inorganic preparations

- (i) Perchlorate salts/cuprous chloride
- (ii) Preparation of Manganese (III) phosphate
- (iii) Preparation of Aluminium potassium sulphate (Potash alum) orChrome alum.

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#### Reference Book:

Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson, 2009.

### CHEM03C6: ORGANIC CHEMISTRY-II

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

## Chemistry of Halogenated Hydrocarbons & Reaction Kinetics:

Alkyl halides: Methods of preparation, nucleophilic substitution reactions  $-S_N1$ ,  $S_N2$  and  $S_Ni$  mechanisms, substrate structure, leaving group, nucleophiles including ambident nucleophiles, substitution involving NGP; relative rate & stereochemical features, nucleophilic substitution vs. elimination.

*Aryl halides:* Preparation, including preparation from diazonium salts, nucleophilic aromatic substitution; S<sub>N</sub>Ar, Benzyne mechanism.

Relative reactivity of alkyl, allyl/benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.



#### Reference Books:

- Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Graham Solomons, T.W. Organic Chemistry, John Wiley & Sons, Inc.
- McMurry, J.E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition, 2013.

### CHEMISTRY PRACTICAL - C6 LAB

## (Credits: Practicals-02, 60 Lectures, Full Marks: 30)

- 1. Functional group tests for alcohols, phenols, carbonyl and carboxylic acid group.
- 2. Organic preparations:
  - i. Acetylation of one of the following compounds: amines (aniline, o-, m-, p- toluidines and o-, m-, p- anisidine) and phenols ( $\beta$ -naphthol, vanillin, salicylic acid) by any one method:
    - a. Using conventional method.
    - b. Using green approach
  - ii. Benzolyation of one of the following amines (aniline, o-, m-, p- toluidines and o-, m-, p-anisidine) and one of the following phenols (β-naphthol, resorcinol, pcresol) by Schötten-Baümann reaction.
  - iii. Oxidation of ethanol/isopropanol (Iodoform reaction).
  - iv. Bromination of any one of the following:
    - a. Acetanilide by conventional methods
    - b. Acetanilide using green approach (Bromate-bromide method)
  - v. Nitration of any one of the following:
    - a. Acetanilide/nitrobenzene by conventional method
    - b. Salicylic acid by green approach (using ceric ammonium nitrate).
  - vi. Selective reduction of *meta*-dinitrobenzene to *m*-nitroaniline.
  - vii. Reduction of p-nitrobenzaldehyde by sodium borohydride.
  - viii. Hydrolysis of amides and esters.
  - ix. Semicarbazone of any one of the following compounds: acetone, ethyl methyl ketone, cyclohexanone, benzaldehyde.
  - x. S-Benzylisothiouronium salt of one each of water soluble and water insoluble acids (benzoic acid, oxalic acid, phenyl acetic acid and phthalic acid).
  - xi. Aldol condensation using either conventional or green method.

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## Course No. CHEM 0891 (FM = 50; C = 4) Organic Practical

Separation of binary mixtures of solid-solid/liquid-solid/liquid-liquid organic compounds and identification of individual components by chemical and spectroscopic methods.

## Course No. CHEM 0892 (FM = 50; C = 4) Computer Application

Introduction to programming languages; basic numerical analysis: solution of nonlinear equations using Newton-Raphson method (e.g. finding the roots of a cubic equation – vander Waals equation), solution of linear systems using Gaussian elimination, interpolation, numerical integration (trapezoidal and Simpson's 1/3<sup>rd</sup> rule), numerical solution of differential equations (Euler and Runge-Kutta method). Fourier transformations and applications in spectroscopy.

Use of molecular geometry optimisation software (Gaussian 09); construction of z-matrix and concept of force field.

Classical Molecular Dynamics (MD) simulation and application to simple systems like Lennard-Jones fluids.

[Effort should be made to reproduce data reported in the literature using the above mentioned numerical methods wherever possible.]

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## CHEMISTRY-DSE 3 and 4 (ELECTIVES)

Credit: 4 + 2

## CHEM06DSE:

# 7. FLUORESCENCE STUDY FOR THE SENSING AND MACROMOLECULAR INTERACTIONS

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Basic idea of spectral intensities: Fermi Golden rule and selection rules from quantum mechanical view points. Potential energy curves, mirror-image symmetry, deactivation – internal conversion and intersystem crossing, radiationless deactivation, Quenching of fluorescence, Stern-Volmer equation and plot, static and dynamic quenching, Life-time variation in presence of quencher. Fluorescence quenching study of tryptophan in protein for the sensing of organic molecules, partial accessibility of tryptophan – modified Stern Volmer plot, study of different folding states. Protein – surfactant interaction, protein – polymer interaction and protein – DNA interaction.

Excimers and exciplexes. Intermolecular energy transfer (FRET). Energy transfer and conformation distributions of biopolymers.

Principles of LASER and characteristic features.

Preliminary ideas of absorption and fluorescence spectrophotometer. Basic ideas of dynamics namely TCSPC, up-conversion and pump-probe techniques.

## Reference Book:

Principles of Fluorescence Spectroscopy. 3rd edition, Joseph R. Lakowicz.

# DSE LAB: FLUORESCENCE STUDY FOR THE SENSING AND MACROMOLECULAR INTERACTIONS

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

- 1. Fluorescence quenching of organic fluorophores
- 2. Fluorescence quenching of tryptophan in different folding states of protein
- 3. Sensing of organic molecules by protein fluorescence study
- 4. FRET for suitable donor acceptor pair
- 5. Protein fluorescence in presence of surfactants, polymers

8. Seminar / Review / Grand Viva

(Credits: Theory-04, Practicals-02, Full Marks-100)

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## Course No. CHEM 1003 (FM = 50; C = 4) Seminar/Review and Grand Viva

**Course Objective:** To provide training on the scientific presentation and group discussion skills which will help them to prepare for job interviews in academia and industries.

- 1. Poster presentation/Seminar/Review (M = 30)
- 2. Grand viva (M = 20)

Course learning outcomes: On completion of the course, the students should be able to

- 1. Present scientific topics in an organized manner
- 2. face the job interviews in a confident manner.

# Course No. CHEM 1091 & CHEM 1092 (FM = 50 + 50) Project dissertation, presentation, defense and proposal

**Course Objective:** To provide training for literature survey, experimental and theoretical research work, instrumental techniques and their operational procedure useful for their employability in industry and academia and also to orient them for future PhD programs.

# Course No. CHEM 1091 (FM=50)

## Project dissertation

The students will be carrying out a project work of 4 months duration in any of the research laboratory in the Department of chemistry according to their interest and availability of the position. This dissertation has to be submitted in the form of a thesis. The M. Sc. thesis will have two chapters. The chapter 1 will contain detail literature survey on the project topic and chapter 2 will contain the origin of the project work, methodology, results and discussion and conclusions. The training and the M. Sc. thesis of these students will then be evaluated.

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