St. Xavier's College – Autonomous

Mumbai

Syllabus for 5th Semester Course in Chemistry (June 2016 onwards)

CONTENTS: THEORY SYLLABUS FOR COURSES:

SYLLABUS UNDER AUTONOMY
CHEMISTRY

SEMESTER V **COURSE: S.CHE.5.01**

SPECTROSCOPY, MOLECULAR & NUCLEAR DYNAMICS [60 LECTURES]

LEARNING OBJECTIVES

1. To encourage students to learn, integrate & analyze the concepts relevant to physical chemistry at the graduation level.

2. To understand the underlying principles of various types of spectroscopy, the rules governing their transitions & their utility in determination of bond length of diatomic molecules & elucidating structures of molecules.

3. To acquire knowledge about methods of detection of various ionizing radioactive radiations, various types of nuclear reactions & nuclear reactors.

4. To understand the basics of quantum chemistry & appreciate the concept of entropy as a probability factor.

5. To learn about basic laws governing photochemical reactions & understand the basic principles of fluorescence, phosphorescence & chemiluminescence.

UNIT I: SPECTROSCOPY (15 L)

1.1: Molecular Spectroscopy

1.1.1: Dipole moment: Polarization of a bond, bond moment, dipole moment and Molecular structure.

1.1.2 Rotational / Microwave Spectroscopy: Rotational spectrum of a diatomic molecule, rigid rotor, moment of inertia, energy levels, limitations of rotational spectra, selection rule, nature of spectrum, determination of inter nuclear distance and isotopic shift.

1.1.3: Vibrational (IR) Spectroscopy: Vibrational motion, degrees of freedom, modes of vibration, vibrational spectrum of a diatomic molecule, simple harmonic oscillator, energy levels, zero point energy, conditions for obtaining vibrational spectrum, selection rule, nature of spectrum. Anharmonic Oscillator : energy levels, selection rule, fundamental band, overtones.

1.1.4: Vibration-Rotation Spectroscopy of diatomic molecules: Vibrating rotor, energy levels, selection rule, nature of spectrum, R and P branches, applications of vibration-rotation spectrum: (i) Force constant, determination and significance (ii) determination of inter-nuclear distance, isotopic shift. Introduction to infrared spectra of simple molecules like H_2O and CO_2.

1.1.5: Raman Spectroscopy: Scattering of electromagnetic radiation, Rayleigh scattering, Raman scattering, nature of Raman spectrum , Stoke's lines, anti-Stoke's lines, Raman shift, quantum theory of Raman scattering, comparative study of IR and Raman spectra, rule of mutual exclusion (example of CO_2 molecule).

UNIT II **(15 L)**

2.1: Nuclear Magnetic Resonance Spectroscopy **(7 L)**

2.1.1: Nuclear spin, magnetic moment, nuclear 'g' factor, energy levels, Larmor precession. Relaxation processes in NMR (spin-spin relaxation and spin-lattice relaxation),

2.1.2: NMR spectrometer, chemical shift, shielding and de-shielding of protons, low resolution NMR spectrum of methanol and ethanol, fine structure of NMR - nuclear spin-spin interaction with reference to methanol and ethanol.

2.2: Electron Spin Resonance Spectroscopy (introductory concepts) **(3 L)**

2.2.1: Derivative curves & g-values, Hyperfine splitting with respect to methyl radical and benzene radical.

2.2.2: Applications of ESR Spectroscopy.

2.3: Mass Spectrometry **(5 L)**

2.3.1: Basic Principles of mass spectrometry, Molecular ion peak, base peak, metastable peak & their uses, nitrogen rule, fragmentation.

2.3.2: Instrumentation, determination of molecular formulae with example, mass spectrum of simple organic compounds e.g., alkanes.

(Numerical problems expected in the above topics)

UNIT III: Molecular & Nuclear Dynamics **(15 L)**

3.1: Nuclear Chemistry

3.1.1: Types of nuclear radiations and their characteristics, behaviour of ion-pairs in electric field, detection and measurement of nuclear radiations using G.M. counter and scintillation counter.

3.1.2: Kinetics of radioactive decay, units of radioactivity (Curie, Becquerel, Rutherford).

3.1.3: Radioactive equilibrium (secular and transient) Determination of radioactive constants for radio-elements having (i) moderate half -life (ii) long half -life (iii) extremely long or short half -life.

3.1.4: Use of radioisotopes as tracers in (i) chemical investigations - reaction mechanism (ii) Age determination – dating by tritium content and by Carbon-14.

3.1.5: Nuclear Reactions: nuclear transmutation, artificial radioactivity (suitable examples using different projectiles are expected.), Q-value of nuclear reaction threshold energy.

3.1.6: Fissile and fertile material, nuclear fission, chain reaction, factors controlling fission process (multiplication factor and critical size or mass of fissionable material), nuclear power reactor and breeder reactor.

3.1.7: Nuclear fusion, characteristics of nuclear fusion, thermonuclear reactions occurring in stellar bodies.

UNIT IV **(15 L)**

4.1: Basics of Quantum Chemistry **(9 L)**

4.1.1: Classical mechanics, limitations of classical mechanics, Black body radiation, photoelectric effect, Compton Effect.

4.1.2: Introduction to quantum theory, Planck's theory of quantization, wave particle dualism, de-Broglie equation, Heisenberg's uncertainty principle. Simple numerical problems.

4.1.3: Progressive and standing waves, boundary conditions, Schrödinger's time independent wave equation, interpretation and properties of wave function.

4.1.4: State function (wave function) and its significance. Concept of operators: definition, addition, subtraction and multiplication of operators, commutative and non-commutative operators, linear operator, position, momentum and energy operators. Eigen function and eigen value, eigen value equation.

4.2: Third Law of Thermodynamics **(3 L)**

4.2.1: Entropy & probability: recapitulation

4.2.2: Statement of Third Law of Thermodynamics

4.2.3: Absolute entropy of solids, liquids & gases.

4.3: Photochemistry **(3 L)**

4.3.1: Laws of Photochemistry, Jablonski energy level diagram – primary & secondary Photochemical processes.

4.3.2: Radiationless transition – internal conversion & intersystem crossing.

4.3.3: Radiative transitions – fluorescence , relation to structure. Phosphorescence- conditions for phosphorescence emission (spin – orbit coupling). Singlet and triplet.

4.3.4: Chemiluminiscence**.**

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CIA I: Short answer questions and numerical problems **20 Marks**

CIA II: Assignment **20 Marks**

Template of Question Paper

SPECTROSCOPY, MOLECULAR & NUCLEAR DYNAMICS COURSE: S.CHE.5.01

OBJECTIVES

UNIT	KNOWLEDGE	UNDERSTANDING	APPLICATION	TOTAL MARKS
I	3	6	6	15
II	3	6	6	15
III	3	6	6	15
IV	3	6	6	15
TOTAL MARKS PER OBJECTIVE	12	24	24	60
% WEIGHTAGE	20	40	40	100

END SEMESTER PAPER PATTERN:

Total Marks: 60 **Maximum Time: 2 hours**

Total number of questions: 4 [all compulsory] of 15 marks each

1 question per unit

Questions set out of 22-23 marks [50% internal choice]

Sub-questions will not exceed 5 marks

SYLLABUS UNDER AUTONOMY
CHEMISTRY

SEMESTER V **COURSE: S.CHE.5.02**

CHEMICAL BONDING AND CO-ORDINATION CHEMISTRY [60 LECTURES]

LEARNING OBJECTIVES

1. To encourage students to analyze and integrate concepts relevant to graduate level Inorganic chemistry.

2. To understand the bond formation of compounds with special reference to MOT and CFT.

3. To build on basic concepts of Co-ordination Chemistry with reference to planar, tetrahedral and octahedral complexes.

4. To study Electronic Spectra of Polyelectronic atoms.

UNIT I: Chemical Bonding (15 L)

1.1: Molecular Symmetry (8 L)

1.1.1: Introduction and Importance.

1.1.2: Symmetry elements and symmetry operations.

1.1.3: Concept of a Point Group with illustrations using the following point groups: (i) $C_{\infty v}$ (HCl) (ii) $D_{\infty h}$ (H_2) (iii) C_{nv}: C_{2v} (H_2O), C_{3v} (NH_3), C_{4v} (iv) C_{nh}: C_{2h} (trans-dichloroethylene) (v) D_{nh}: D_{2h}, D_{3h} (BCl_3), D_{4h} (vi) D_{nd}: D_{2d} (allene), T_d(CH_4) and O_h

1.2: Molecular Orbital Theory for polyatomic species (5 L)

(Prior Knowledge: MOT for diatomic molecules)

1.2.1: Simple triatomic species H_3^+ and H_3 (correlation between bond angle and molecular orbitals)

1.2.2: (i) BeH_2 (ii) H_2O (iii) NH_3 (iv) CH_4 and (v) CO_2

1.3: Metallic Bond (2 L)

1.3.1: Band theory

1.3.2: Explanation of electrical properties of conductors, insulators and semiconductors (n- and p- types) on the basis of Band theory.

UNIT II: Inner Transition Elements (15 L)

2.1: Lanthanide Series (11 L)

2.1.1: Chemistry of lanthanides with reference to i) Occurrence & extraction of Lanthanides (ii) lanthanide contraction (iii) oxidation states (iv) magnetic properties (v) color and spectra (f-f transition spectra) and (vi) complex formation (types and stereochemistry of the complexes).

2.1.2: Separation of lanthanides by (i) ion-exchange and (ii) solvent extraction methods.
Self Study**:** Application of lanthanides.

2.2 Actinide Series (4 L)

2.1.1: Chemistry of Uranium and Plutonium with reference to occurrence, extraction (solvent extraction method), properties and applications.
Self Study**:** i) Applications of actinides.
ii) Comparative chemistry of lanthanides and actinides.

UNIT III: Co-ordination Chemistry (15 L)

3.1: Crystal Field Theory (CFT) (8 L)

3.1.1: Basic tenets of Crystal Field Theory and effect of Crystal Field on central metal valence orbitals

3.1.2: Splitting of d orbitals in octahedral, tetrahedral and square planar complexes and Jahn Teller Effect

3.1.3: Crystal field splitting energy (10Dq/Δo) for octahedral complexes and factors affecting the magnitude of Δo.

3.1.4: Crystal field stabilization energy (CFSE), calculation of CFSE for octahedral and tetrahedral complexes with d_1 to d_{10} metal ion configurations, high-spin and low-spin complexes.

3.1.5: Effect of crystal field splitting on (i) Ionic radius and (ii) Lattice energy.

3.1.6: Experimental evidence for co-valence in co-ordination compounds:

i) ESR spectrum of $[IrCl_6]^{2-}$.

ii) NMR spectrum of tris(acetylacetonato)vanadium(III) complex.

iii) Intensities of d-d transitions and (iv) Nephelauxetic effect.

Self Study: Merits and Demerits of CFT.

3.2: Molecular Orbital Theory (MOT) of Coordination Complexes (4 L)

3.2.1: Application to octahedral complexes in case of (i) $[Ti(H_2O)_6]^{3+}$ (ii) Fluoro complexes of Fe (II) and Co (III) (iii) Cyano complexes of (Fe (III) and ammino complexes of Co (III).

Self Study: Molecular orbital diagram for Fluoro complexes of Fe(III) and Cyano Complexes of Fe (II).

3.2.2: Effect of pi-bonding on ligand field splitting parameter in M→L π- and L→M π-interactions.

3.3 Stability of Octahedral Complexes (3 L)

3.3.1: Thermodynamic stability and kinetic stability of complexes with examples.

3.3.2: Stability constants: stepwise and overall constants and their inter-relationship**.**

3.3.3: Factors affecting thermodynamic stability.

Self Study*:* Method of determination of stability constants.

UNIT 1V: Spectra and Substitution Reactions (15 L)

4.1: Electronic States and Terms of Polyelectronic atoms (4 L)

4.1.1: Introduction: electronic configuration and electronic states, Term symbols, coupling of spin momenta (MS), orbital momenta (ML) and spin orbit coupling or Russell-Saunders coupling.

4.1.2: Determination of Terms for p.p and p^2 electronic configuration (as in a carbon atom), Hund's rule.

4.1.3: Terms and micro-states for transition metal atoms/ions.

4.2: Electronic Spectra (4 L)

4.2.1: Types of electronic transitions like intra-ligand transitions, charge transfer transitions and intra-metal transitions (d-d or ligand field transitions for transition metals).

4.2.2: Rules for electronic transitions: Spin and Orbital or Laporte selection rules.

4.2.3: Splitting of Terms in weak crystal field, the Hole Formalism.

4.2.4: Orgel Diagrams for D Terms (i.e d^1, d^4 , d^6 , d^9 electronic configurations) and their use in interpretation of visible electronic absorption spectra of these configurations.

4.3: Magnetic Properties of Transition Metal Complexes (3 L)

4.3.1: Types of magnetic behavior, methods of determining magnetic susceptibility, spin-only formula, L-S coupling, correlation of μ_s and μ_{eff} values, orbital contribution to magnetic moments and application of magnetic moment data for 3d metal complexes.

4.4. Substitution Reactions in Octahedral Complexes (4 L)

4.4.1: Introduction, types of reactions in complexes.

4.4.2: Ligand substitution reactions: basic mechanism.

4.4.3: Inert and labile complexes and electronic configurations and lability of complexes.

4.4.4: Acid hydrolysis, base hydrolysis and anation reactions.

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CIA I: Short answer questions **20 MARKS**

CIA II: Multiple choice questions **20 MARKS**

Template of Question Paper

CHEMICAL BONDING AND CO-ORDINATION CHEMISTRY COURSE: S.CHE.5.02

OBJECTIVES

UNIT	KNOWLEDGE	UNDERSTANDING	APPLICATION	TOTAL MARKS
I	6	6	3	15
II	6	6	3	15
III	6	6	3	15
IV	6	6	3	15
TOTAL MARKS PER OBJECTIVE	24	24	12	60
% WEIGHTAGE	40	40	20	100

END SEMESTER PAPER PATTERN:

Total Marks: 60 **Maximum Time: 2 hours**

Total number of questions: 4 [all compulsory] of 15 marks each.

1 question per unit.

Questions set out of 25 marks [50% internal choice].

Sub questions will not exceed 5 marks.

SYLLABUS UNDER AUTONOMY
CHEMISTRY

SEMESTER V **COURSE: S.CHE.5.03**

STEREOCHEMISTRY AND NATURAL PRODUCTS [60 LECTURES]

LEARNING OBJECTIVES

1. To consolidate the students' understanding of stereochemistry of the molecules and reactions.
2. To investigate reaction mechanisms.
3. To give the students an overview of biomolecules.

UNIT I: Stereochemistry (15 L)

1.1: Elements of symmetry: Mirror plane, centre (inversion centre), rotation-reflection alternating) axis. **(2 L)**

1.2: Molecular chirality: Compounds without stereogenic centres but with chiral axis: cummulenes, spirans and biphenyls; and with chiral planes: cyclophanes and ansa compounds. Assignment of descriptors - (R,S) nomenclature. **(4 L)**

1.3: Conformational analysis of cyclohexane: Angle, eclipsing and transannular strain in small , medium and large cycloalkanes (4- and 5- membered rings). Mono- and di- alkyl cyclohexanes and their relative stabilities. **(3 L)**

1.4: Stereoselectivity and stereospecificity: Idea of enantioselectivity (*ee*) and diastereoselectivity (*de*). Topicity – enantiotopic and diastereotopic ligands and faces. **(1 L)**

1.5: Stereochemistry and reaction mechanisms: **(5 L)**

a) Substitution reactions – S_Ni .
b) Elimination reactions - E_1 and E_2.
c) Addition reactions to olefins - i) catalytic hydrogenation ii) bromination iii) syn- hydroxylation with OsO_4 and $KMnO_4$ iv) peroxyacids.

UNIT II: Mechanism of organic reactions (15 L)

2.1: Investigation of reaction mechanisms: Product analysis including crossover products, trapping of intermediates, isotopic labeling, kinetic and stereochemical evidence. **(2 L)**

2.2: Thermodynamic and kinetic control of organic reactions: Concept with mechanisms of the following reactions: Addition of HX to butadiene; sulfonation of naphthalene. Nucleophilicity/electrophilicity v/s Basicity/acidity. **(3 L)**

2.3: Mechanism of reactions of carbonyl compounds with nucleophiles: (5 L)

a) Formation of acetals from aldehydes and ketones.
b) Reaction of aldehydes and ketones with primary and secondary amines.
c) Acyl nucleophilic substitution (tetrahedral mechanism): Acid-catalysed esterification of carboxylic acids and base-promoted hydrolysis of esters.

2.4: Effect of neighbouring group participation (NGP) on organic reactions: (3 L)
For reactions involving groups or substituents like halogen, oxygen, sulphur, phenyl ring, C-C bond of the ring (non-classical carbocations).

2.5: Pericyclic reactions:
[2+2] and [4+2] cycloaddition reactions. **(2 L)**

UNIT III: Natural Products (15 L)

3.1 Introduction: Introduction to natural products with respect to sources and classes. **(1 L)**

3.2: Carbohydrates

3.2.1: Introduction: Sources, Classification , reducing and non-reducing sugars, D and L- notations. **(1 L)**

3.2.2: Structures of Monosaccharides: Open chain structures of aldoses and ketoses, ring structures of aldohexoses, aldopentoses and ketohexoses. **(2 L)**

3.2.3: Determination of open chain configurations of Monosaccharides:
Configuration of D (+) Glucose and D(-) Fructose . **(2 L)**

3.2.4: Stereoisomers of Monosaccharides: (2 L)
Enantiomers and diastereoisomers of monosaccharides, epimers, anomers, mutarotation (with mechanism) in D-Glucose.

3.2.5: Chain lengthening and shortening reactions: (2 L)
Kiliani-Fischer synthesis, Wohl's method.

3.2.6: Reactions of D-Glucose and D-Fructose: (2 L)
(**a**) osazone formation
(**b**) reduction with $NaBH_4$ and Ni / H_2

(**c**) oxidation with bromine water, conc.HNO_3 and HIO_4

(**d**) interconversion of D (+) Glucose to D(-)Fructose and D(-)Fructose to D(+)Glucose

(**e**) acetylation

(**f**) methylation [(**e)** and(**f)** with cyclic pyranose form].

3.2.7: Introduction to disaccharides and structures of sucrose and maltose. **(1 L)**

3.2.8: Glycosides: General structure giving indican as an example. **(2 L)**

UNIT IV: Chemistry of important Biomolecules (15 L)

4.1: Amino acids and Proteins (6 L)

4.1.1: Amino acids: Introduction, Classification, syntheses of amino acids-Strecker synthesis, Amidomalonate synthesis and Erlenmeyer Azalactone synthesis.

4.1.2: Polypeptides : Introduction, peptide bond, Merrifields solid phase peptide synthesis, Bergmann method.

4.1.3: Proteins: Structure of proteins, classification of proteins, properties of proteins, denaturation of proteins, biosynthesis of proteins.

4.1.4: Separation and purification of proteins:
Gel filtration chromatography, electrophoresis.

4.1.5: Catabolism of amino acids: Transamination, oxidative deamination, decarboxylation.

4.2: Nucleic Acids (6 L)

4.2.1: Introduction, classification of nucleic acids.

4.2.2: Structures of sugars and bases in nucleic acids.

4.2.3: Structures of nucleosides and nucleotides in DNA and RNA.

4.2.4: Structure of DNA: Chargaff's rule of DNA configuration, Watson-Crick model of DNA.

4.2.5: Structure of RNA, types of RNA.

4.2.6: DNA replication, mutations, DNA repair.

4.2.7: Transcription, DNA sequencing, polymerase chain reaction and its applications.

4.3: Alkaloids and Terpenoids **(3 L)**

4.3.1: Introduction, functions of alkaloids and terpenoids.

4.3.2: Structure elucidation, synthesis and biological properties of nicotine and citral.

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CIA I: Written test **20 Marks**

CIA II: Models or 3-D representations of molecules with stereochemistry 20 Marks

Template of Question Paper

STEREOCHEMISTRY AND NATURAL PRODUCTS COURSE: S.CHE.5.03

OBJECTIVES

UNIT	KNOWLEDGE	UNDERSTANDING	APPLICATION	TOTAL MARKS
I	5	5	5	15
II	5	5	5	15
III	5	5	5	15
IV	5	5	5	15
TOTAL MARKS PER OBJECTIVE	20	20	20	60
% WEIGHTAGE	33	34	33	100

END SEMESTER PAPER PATTERN:

Total Marks: 60 **Maximum Time: 2 hours**

Total number of questions: 4 [all compulsory] of 15 marks each

1 question per unit

Questions set out of 22-23 marks [50% internal choice]

Sub-questions will not exceed 5 marks

SYLLABUS UNDER AUTONOMY
CHEMISTRY

SEMESTER V **COURSE: S.CHE.5.04**

GENERAL ANALYTICAL AND PHARMACEUTICAL CHEMISTRY

[60 LECTURES]

LEARNING OBJECTIVES

1. To understand sources of errors in measurement.
2. To promote an understanding about data collection, manipulation and interpretation.
3. To expose students to commonly used sampling techniques.
4. To understand the principles involved in titrimetric analysis.
5. To give the students a knowledge of non-aqueous titration.
6. To comprehend the principles and instrumental techniques involved in chromatography and solvent extraction.
7. To motivate students to solve numerical problems.
8. To familiarize the students with different concepts in pharmaceutical chemistry.
9. To bridge the gap between academics and industry.

UNIT I: Treatment of Analytical Data-I and Sampling (15 L)

1.1: Treatment of Analytical Data-I (7 L)

1.1.1: Types of errors, determinate and indeterminate errors, minimization of errors, constant and proportionate errors.

1.1.2: Accuracy and precision, measures of dispersion and central tendency: mean, median, average deviation, relative average deviation, standard deviation, variance, coefficient of variation (Numerical problems expected).

1.2: Sampling (8 L)

1.2.1: Sampling techniques, equipments used in sampling of gases.

1.2.2: Methods and equipments used in sampling of homogeneous and heterogeneous liquids, sampling of static and flowing liquids.

1.2.3: Samplers used in sampling of solids, importance of particle size and sample size, method of reduction in sample size. Collection, preservation and dissolution of the sample.

1.2.4: Self Study: Terms involved in sampling, importance and objectives of sampling.

UNIT II: Titrimetric Analysis (15 L)

2.1: Precipitation titrations: Argentimetric titrations, construction of the titration curves, detection of end point by (i) Mohr's method (ii) Volhard's method (iii) using adsorption indicators, theory and applications.

2.2: Complexometric titrations: General introduction, EDTA titrations, advantages and limitations of EDTA as the titrant, absolute and conditional formation constants of metal- EDTA complexes, Construction of titration curves, types of EDTA titrations, methods of increasing the selectivity of EDTA as a titrant, metallochromic indicators, theory and applications.

2.3: Redox titrations: General introduction, theory of redox indicators, construction of the titration curves in the case of (i) Fe (II) vs. Ce(IV) (ii) Fe(II) vs. dichromate. Use of diphenyl amine and ferroin as redox indicators.

2.4: Nonaqueous titration: Need for non-aqueous titration, basic principle, requirement of solvent, types of solvents, solvents used in non-aqueous titration and end point detection, applications.

2.5: Self Study: Acid –base titrations: Construction of titration curves and choice of indicators in the titration of : (i) strong acid and strong base (ii) strong acid and weak base (iii) weak acid and strong base (iv) weak acid and weak base.

UNIT III: Separation Techniques-1 (15 L)

3.1: Solvent extraction: Role of complexing agents in solvent extraction, chelation, Ion pair formation, solvation, types of **solvent extraction**: batch, continuous

3.2: Planar chromatography: Principle, techniques and applications of Paper Chromatography and Thin layer chromatography.

3.3: Principle, instrumentation and applications of **Gas Chromatography and High Performance Liquid Chromatography.**

3.4: Supercritical fluid chromatography: Introduction, supercritical fluid choice, their properties, instrumentation and applications.

3.5: Electro-chromatography: Electrophoresis.

3.6: Self Study: Introduction to chromatographic techniques, basic principles, classification of Chromatographic techniques**.**

UNIT IV: **Introduction to Pharmaceutical Chemistry-1 (15 L)**

4.1: Introduction to pharmaceutical chemistry, TQM, concept of Quality, Quality Control, Quality Assurance and their inter-relation.

4.2: Concept of FDA, their role and importance, classification of drugs according to FDA

Pharmacopoeia: History, Drug act and schedules, components of pharmacopoeia.

4.3: Good Laboratory Practices [GLP], ISO series.

4.4: Good Manufacturing Practice [GMP], Drug Technical Advisory Board [DTAB].

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1. **D. A. Skoog, D.M.West, F.J. Holler,** Fundamantals of Analytical Chemistry, 8th ed. Philadelphia, Saunders College Publishing, 1996.
2. **D. A. Skoog, F.J.Holler, T.A.Nieman,** Principles of Instrumental Analysis, 6th ed. Philadelphia, Saunders College Publishing, 1996.
3. **G.D.Christian,** Analytical Chemistry, 6th ed. John Wiley &Sons, Singapore, 2004.
4. **J.G.Dick,** Analytical Chemistry, International Student's Edition, McGraw Hill, Kogakusha Limited, New Delhi, 1973.
5. **R.A.Dey & D.L.Underwood,** Quantitative Analysis, 6th ed. Prentice Hall Of India Pvt. Ltd. New Delhi, 1993.
6. **M.Valcarcel,** Principles Of Analytical Chemistry, Springer International Edition, Berlin, 2000.
7. **E.Prichard, & V. Barwick,** Quality Assurance in Analytical Chemistry, Wiley.
8. **S. M. Khopkar,** Basic Concepts of Analytical Chemistry, 3rd ed, New Age International Publishers, 2008.
9. **S. M. Khopkar,** Analytical Chemistry Problems and Solutions, New Age International Publishers, 2002.
10. **A. I. Vogel,** Textbook of Quantitative Chemical Analysis, 6th ed, Pearson Education, 2002.
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12. **J. M. Miller,** Separation methods in Chemical Analysis, John Wiley, 1975.
13. **J. A. Dean,** Chemical Separation Methods,1969.
14. **R.D. Braun,** Introduction to Instrumental methods of Analysis, McGraw Hill, 1987.
15. **G. R. Chatwal and S. K. Anand**: Instrumental methods of Chemical Analysis, Himalaya Publishing House.
16. **H. H. Willard, L. L. Merritt and J. A. Dean**; Instrumental methods of Analysis, 7th ed. CBS Publishers, 1986.
17. **A. H. Beckett and J. B. Stenlake: Practical Pharmaceutical Chemistry,** 4th ed. Part I and II.

18. R. J. Hamilton and P.A.Sewell: Introduction to HPLC, 2nd edition.

19. Ashutosh Kar ; Pharmaceutical Drug Analysis.

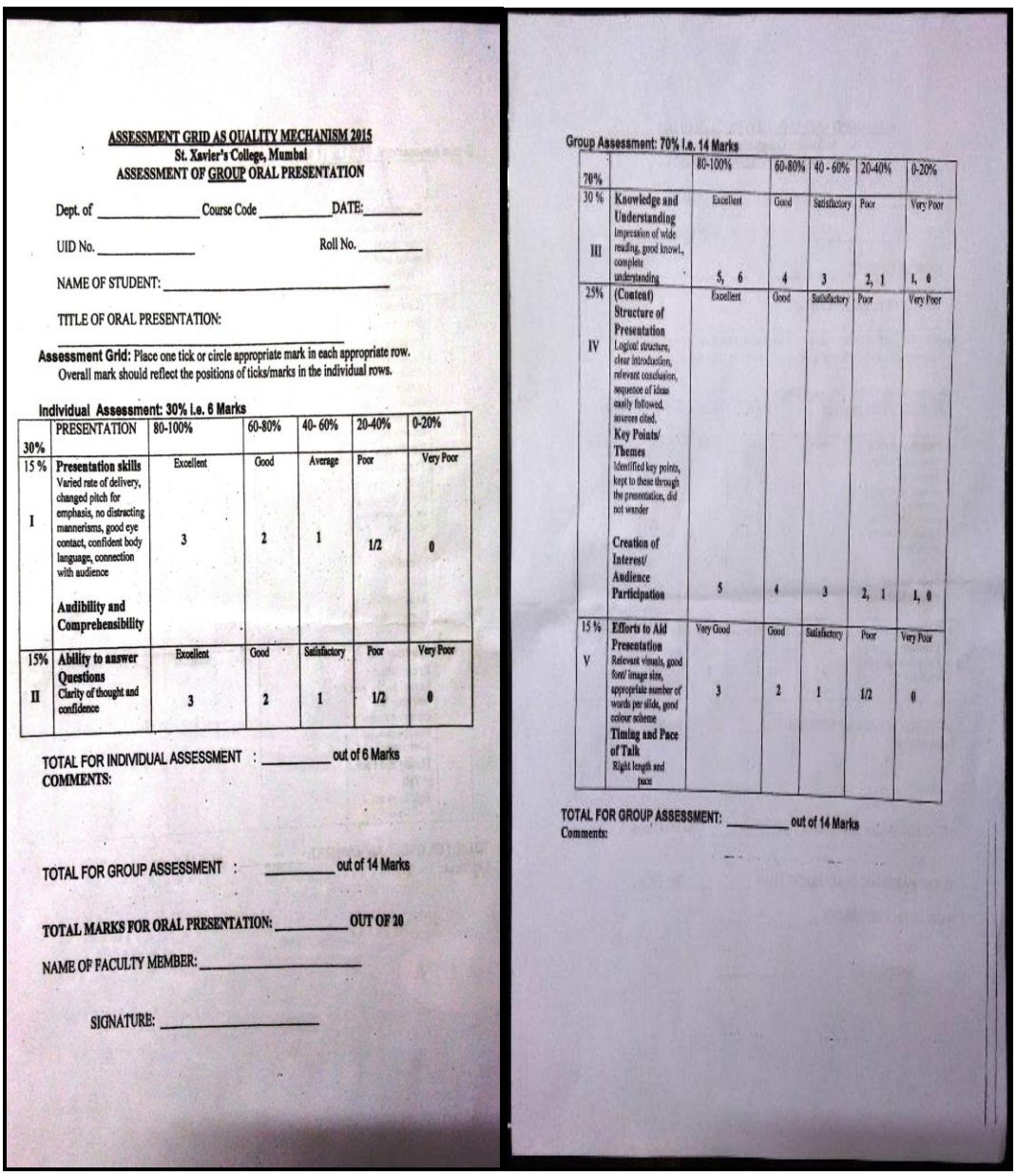
20. A. M. Bond, Anal. Chim. Acta 62, 415 (1972).

21. F. Elizabeth Prichard, Quality in the Analytical Chemistry Laboratory.

CIA I: Short answer questions **20 MARKS**

CIA II: Oral Presentation **20 MARKS**

❖ ASSESSMENT GRID FOR ORAL PRESENTATION



ASSESSMENT GRID AS QUALITY MECHANISM 2015
St. Xavier's College, Mumbai
ASSESSMENT OF GROUP ORAL PRESENTATION

Dept. of _____ Course Code _____ DATE:_____

UID No. _____ Roll No. _____

NAME OF STUDENT: _____

TITLE OF ORAL PRESENTATION:
_____

Assessment Grid: Place one tick or circle appropriate mark in each appropriate row.
Overall mark should reflect the positions of ticks/marks in the individual rows.

Individual Assessment: 30% i.e. 6 Marks

30%	PRESENTATION	80-100%	60-80%	40- 60%	20-40%	0-20%
15 % I	**Presentation skills** Varied rate of delivery, changed pitch for emphasis, no distracting mannerisms, good eye contact, confident body language, connection with audience **Audibility and Comprehensibility**	Excellent 3	Good 2	Average 1	Poor 1/2	Very Poor 0
15% II	**Ability to answer Questions** Clarity of thought and confidence	Excellent 3	Good 2	Satisfactory 1	Poor 1/2	Very Poor 0

TOTAL FOR INDIVIDUAL ASSESSMENT : _____ out of 6 Marks
COMMENTS:

TOTAL FOR GROUP ASSESSMENT : _____ out of 14 Marks

TOTAL MARKS FOR ORAL PRESENTATION: _____ OUT OF 20

NAME OF FACULTY MEMBER: _____

SIGNATURE: _____

Group Assessment: 70% i.e. 14 Marks

70%		80-100%	60-80%	40 - 60%	20-40%	0-20%
30 % III	**Knowledge and Understanding** Impression of wide reading, good knowl., complete understanding	Excellent 5, 6	Good 4	Satisfactory 3	Poor 2, 1	Very Poor 1, 0
25% IV	**(Content) Structure of Presentation** Logical structure, clear introduction, relevant conclusion, sequence of ideas easily followed, sources cited. **Key Points/ Themes** Identified key points, kept to these through the presentation, did not wander **Creation of Interest/ Audience Participation** 5	Excellent	Good 4	Satisfactory 3	Poor 2, 1	Very Poor 1, 0
15 % V	**Efforts to Aid Presentation** Relevant visuals, good font/ image size, appropriate number of words per slide, good colour scheme **Timing and Pace of Talk** Right length and pace	Very Good 3	Good 2	Satisfactory 1	Poor 1/2	Very Poor 0

TOTAL FOR GROUP ASSESSMENT: _____ out of 14 Marks
Comments:

Template Of Question Paper

GENERAL ANALYTICAL AND PHARMACEUTICAL CHEMISTRY:

COURSE: S.CHE.5.04

OBJECTIVES

UNIT	KNOWLEDGE	UNDERSTANDING	APPLICATION	TOTAL MARKS
I	4-5	5-6	5-6	15
II	4-5	5-6	5-6	15
III	4-5	5-6	5-6	15
IV	4-5	5-6	5-6	15
TOTAL MARKS PER OBJECTIVE	16-20	20-24	20-24	60
% WEIGHTAGE	27-34	34-40	34-40	100

END SEMESTER PAPER PATTERN:

Total Marks: 60 **Maximum Time: 2 hours**

Total number of questions: 4 [all compulsory] of 15 marks each.

1 question per unit.

Questions set out of 22-23 marks [50 % internal choice]

Sub questions will not exceed 5 marks

PRACTICAL CHEMISTRY **COURSE: S.CHE.5.PR**

LEARNING OBJECTIVES

1. **To learn to perform instrument based experiments and non-instrumental experiments with correct techniques.**
2. **To develop skills of observation, recording and analyzing data.**
3. **To learn to present the experimental work in a systematic manner.**

PHYSICAL CHEMISTRY: COURSE 1

INSTRUMENTAL EXPERIMENTS

A. POTENTIOMETRY

1. To determine the pK_a value of a given weak monobasic acid (CH_3COOH) by e.m.f. measurements using Quinhydrone electrode.

2. To determine solubility product and solubility of silver chloride potentiometrically using chemical cell.

3. To determine solubility product and solubility of silver chloride potentiometrically using concentration cell.

4. To determine electrode potential of saturated calomel electrode at room temperature and using this value to determine standard potential of Ag^+ | Ag electrode.

5. To determine the amount of Fe (II) and formal redox potential in the given solution by potentiometric titration against a standard solution of potassium dichromate.

B. CONDUCTOMETRY

6. To determine the relative strength of monochloroacetic acid and acetic acid conductometrically.

7. To determine the strength of a given dibasic acid by conductometric titration.

C. POLARIMETRY

8. To determine the specific rotation of glucose / cane sugar.

D. SPECTROPHOTOMETRY

9. To verify Beer-Lambert's law using potassium dichromate / potassium permanganate solution & hence determine its molar absorptivity.

E. pH METRY

10. To determine the acidic and basic dissociation constants of an amino acid and its iso-electric point.

INORGANIC CHEMISTRY: COURSE 2

INSTRUMENTAL

INORGANIC PREPARATIONS

TITRIMETRIC ANALYSIS

1. Instrumental

i) To study the complex formation between Fe(III) and salicylic acid, find the formula and stability constant of the complex using colorimeter.
ii) To determine the strength of unknown KCl, KBr and KI solutions in a mixture of all three potentiometrically when titrated against N/10 $AgNO_3$ solution.

2. Inorganic Preparations

i) Tris-(ethylenediamine)nickel(II)thiosulphate.
ii) Bis-(acetylacetonato) copper(II).
iii) Bis-8-hydroxyquinolato magnesium(II).
iv) Potassium trioxalato chromate (III).

3. Titrimetric analysis

i) Determination of metal content in Tris(ethylenediamine)nickel(II)thiosulphate.
ii) Determination of metal content in Bis(acetylacetonato) copper(II).
iii)Determination of metal content in Bis-8-hydroxyquinolato magnesium(II).
iv)Determination of metal content and oxalate ions in Potassium trioxalato chromate (III)

ORGANIC CHEMISTRY: COURSE 3

A. Organic Separation

Separation of a binary mixture: Type of mixture, Separation and Identification (microscale) of both the components through systematic scheme of identification.
Type: Solid + Solid (no carbohydrates to be given)
Mass of solid: 3—4 g.

B. Preparation of organic compounds

Preparation of organic compound as per the procedure given. Measuring the mass of crude, purification of the separated product by crystallisation and recording of the m.p.
Quantity of the reactant to be given: 1 g.

Preparations:

1. 2- Naphthol to Methyl-2-naphthyl ether
2. Hydroquinone / 2-Naphthol to Acetate
3. Phthalic anhydride to Phthalimide
4. Glucose to Glucosazone

C. Green Chemistry: Demonstration Experiments

1. Benzil-benzylic acid rearrangement.

2. Pechmann condensation in Coumarin synthesis.

Note: A minimum of **six** mixtures and four preparations should be covered in the Semester.

ANALYTICAL CHEMISTRY: COURSE 4

NON-INSTRUMENTAL EXPERIMENTS

1. Estimation of persulphate in the given sample by the method of back titration.

2. Determination of the calcium and magnesium content of a Dolomite sample.

3. Determination of glucose content in a honey sample by Willstatter's method.

4. Determination of Vitamin C by titration with potassium bromate.

5. Determination of dissolved oxygen in the given water sample.

6. Determination of Iodine value by Wij's method for the given oil sample.

7. Thin layer chromatographic separation of organic compound.

8. Chemical Oxygen Demand (COD) of water sample.

9. Determination of salinity of the given water sample.

10. Estimation of drug by non-aqueous titration.

REFERENCES:

1. **O.P Pandey, D. N. Bajpai and S. Giri,** *Practical Chemistry*, Delhi: S. Chand, 2008.

2. **V. D.Athawale and P. Mathur,** Experimental Physical Chemistry: New Age International. 2008.

3. **H. N. Patel, S.P.Turakhia, S. S. Kelkar, and S.R. Puniyani,** Post Graduate Practical Chemistry, Himalaya Publishing House, 2012.

❖ CIA AND END SEMESTER PRACTICAL EXAMINATION

Course 1: Physical Chemistry – Instrumental Experiment.

Course 2: Inorganic Chemistry – Instrumentation, Inorganic Preparation and Estimation.

Course 3: Organic Chemistry – Separation and Identification of solid-solid mixture.

Course 4: Analytical Chemistry – Non-instrumental Experiment.

Journal: 5 marks per course.

CIA: 15 marks per course.

Duration: 4 periods to be conducted during regular practicals by the Faculty-in- charge. One or more practical skills will be tested in the CIA.

End Semester Examination: 30 marks per course. This includes a 5 mark viva-voce based on the theory behind all the experiments conducted per course.

There will be an External Examiner and an Internal Examiner responsible for two courses each.

Duration: 3½ hrs per course.

Batch size: Max 20 students per batch for courses 2 and 3 and 10 students per batch for courses 1 and 4 (involving instruments).

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SYLLABUS UNDER AUTONOMY
CHEMISTRY

SEMESTER V **COURSE NO.: S.CHE.5.AC**

DRUGS AND COLOR CHEMISTRY **[60 LECTURES]**

Learning Objectives

1) To familiarize students with the mode of action of drugs.
2) To understand the uses and the side effects of certain drugs for various diseases.
3) To study the synthesis of different drugs
4) To study the nomenclature and characteristics of dyes.
5) To study the concept of colour and its relation to chemical structure.
6) To familiarize the students with the types of fibres, application of dyes and how the dyes are attached to them.
7) To familiarize the students with the syntheses of some representative dyes.
8) To create an awareness of the current concern about the toxicity of dyes and their effect on ecology.

1. 1: General Introduction to Drugs (6 L)

1.1.1: Definition of a drug, requirements of an ideal drug, classification of drugs (based on therapeutic action).
1.1.2: Nomenclature of drugs: Generic name, Brand name, Systematic name.
1.1.3: Definition of the following medicinal terms: Pharmacon, Pharmacophore, Prodrug, Half-life efficiency, LD_{50}, ED_{50}, Therapeutic Index.
1.1.4: Brief idea of the following terms: Receptors, Drug-receptor interaction, Drug Potency, Bioavailability, Drug toxicity, Drug addiction, Spurious Drugs, Misbranded Drugs, Adulterated Drugs, Pharmacopoeia.

1.2: Routes of Drug Administration and Dosage Forms (2 L)

1.2.1: Oral and Parenteral routes with advantages and disadvantages.
1.2.2: Formulations, Different dosage forms (emphasis on sustained release formulations.)

1.3: Pharmacodynamic agents

A brief introduction of the following pharmacodynamic agents and the study with respect to their chemical structure, chemical class, therapeutic uses and side effects.

1.3.1: CNS Drugs (5 L)

Classification based on pharmacological actions, concept of sedation and hypnosis, anaesthesia. Phenobarbitone (Barbiturates), Phenytoin, (Hydantoins), Trimethadione (Oxazolidinediones), Piracetam (Pyranones), Midazolam, Alprazolam (Benzodiazepines), Methylphenidate (Piperidines), Chlorpromazine (Phenothiazines), Fluoxetine (Phenyl propyl amines). Synthesis of Trimethadione, Methylphenidate, Phenytoin.

1.3.2: Analgesics and Antipyretics (2 L)

Morphine (Phenanthrene alkaloids), Tramadol (Cyclohexanols), Aspirin (Salicylates), Paracetamol (p-Aminophenols). Synthesis of Tramadol, Paracetamol.

2.1: Anti-inflammatory Drugs (2 L)

Mechanism of inflammation and various inflammatory conditions. Prednisolone, Betamethasone (Steroids), Aceclofenac (N- Aryl anthranilic acids), Mefenamic Acid (N-Aryl anthranilic acids). Synthesis of Aceclofenac.

2.2: Antihistaminic Drugs (2 L)

Mechanism of histamine release & its action. Diphenhydramine (ethanolamines), Cetrizene (piperazine), Chloropheniramine maleate (ethyl amines),Omeprazol, Pantoprazole (Benzimidazoles). Synthesis of cetirizine.

2.3: Cardiovascular Drugs (3 L)

Classification based on pharmacological action.
Enalapril (alpha -amino acids), Isosorbide dinitrate (Nitrates),
Atenolol (Aryloxy propanol amines), Nifedipine (Pyridines), Chlorthiazide (Thiazides),Frusemide /Furosemide (Sulfamyl benzoic acid), Spironolactone (Steroidal- 17- gamma-lactones). Synthesis of Furosemide,
Atenolol from 3-Hydroxy phenyl acetamide.

2.4: Anti-diabetic Agents (2 L)

General idea and types of diabetes; Insulin therapy Glibenclamide (sulphonyl ureas), Metformin (Biguanides).

2.5: Antiparkinsonism Drugs (2 L)

Idea of Parkinson's disease, Procyclidine hydrochloride (Pyrrolidines), Ethopropazine hydrochloride (Phenothiazines), Laevodopa (alpha -amino acids). Synthesis of Levodopa from Vanillin.

2.6: Drugs for Respiratory System (2 L)

General idea of Expectorants: Mucolytes; Bronchodilators, Decongestants and Antitussives, Bromhexine (Phenyl methyl amines), Salbutamol, Pseudo- ephedrine (Phenyl ethyl amines), Oxymetazoline (Imidazolines), Codeine Phosphate (Opiates). Synthesis of Salbutamol.

2.7: Mode of Action of the Following Drugs (2 L)

Barbiturates (As sedatives and hypnotics), Atenolol (As β-1 blocker), Diphenhydramine (As Anthistaminic agent), Glibenclamide (As oral hypoglycemic agent).

3.1: INTRODUCTION TO DYESTUFF CHEMISTRY (5 L)

3.1.1: Important landmark in the history of dyes

3.1.1.1: Natural colouring matter and their limitations: e.g,; Heena, Turmeric, Kesar, Chlorolphyll, Indigo, Alizarine from roots of madder plants, Logwood, Tyrian Purple.

3.1.1.2: Synthetic Dyes: Important milestones i.e. Mauve, Diazotization of aniline, Congo Red, Synthesis and structure of Indigo, Disperse Dye, Fluorescent Brighteners, Procion Reactive Dyes, Remazole Dyes. (Emphasis on Name of the Scientist and the year of discovery is required). Structure is not expected.

3.1.2: Definition of dyes, Properties i.e. Colour, Chromophore and Auxochrome, Solubility, Linearity, Coplanarity, Fastness Properties, Substantivity, Economic Viability.

3.1.3: Explanation of nomenclature of commercial dyes with atleast one example, suffixes-G, O, R, B, 6B, GK, 3GK, 6GK, L, S. Explanation: naming of dyes by colour index(two examples).

3.2: Classification Of Dyes Based On Constitution (3 L)

(Examples are mentioned below with structures)

(i) Nitro Dyes-Naphthol yellow S

(ii) Nitroso Dye-Gambine Y

(iii) Azo Dyes- (a) Monoazo Dyes- Metanil yellow
(b) Diazo Dyes- Napthol Blue Black
(c) Triazo Dyes - Chloroamine Green B

(iv) Diphenymethane Dyes-Auramine O

(v) Triphenyl methane Dyes
(a) Malachite Green Series- Naphthalene Green V
(b) Magenta Series- Acid Magenta
(c) Rosolic acid Series-Chrome Violet

(vi) Heterocyclic Dyes
(a) Xanthene-Rhodamine 6G
(b) Acridines-Acriflavine
(c) Azines- Safranine B
(d) Oxazines-Capri blue,
(e) Thiazines-Methylene Green
(f) Quiolines- Quinoline Yellow
(g) Thiazoles-Primuline

(vii) Benzoquinones and Naphthaquinones- Napthazarin

(viii) Anthraquinone Dyes- Indanthrene, Turquoise Blue 3GK

(ix) Indigoids-Indigo Caramine

(x) Pthalocyanines-Sirius Light Green FFGL

3.3: Classification Based on Application (6 L)

Definition, fastness properties & applicability on substrates examples with structures

(a) Acid Dyes- Orange II
(b) Basic Dyes-Methyl Violet, Victoria Blue B
(c) Direct Cotton Dyes- Benzofast Yellow 5GL
(d) Azoic Dyes-Diazo components; Fast yellow G, Fast orange R. Coupling components. Naphthol AS, Naphthol ASG
(e) Mordant Dyes-Eriochrome Black A, Alizarin.
(f) Vat Dyes- Indanthrene Brown RRD, Indanthrene Red 5GK.
(g) Sulphur Dyes- Sulphur Black T (no structure)
(h) Disperse Dyes-Celliton Fast Brown 3R, Perlon Fast Blue FFR
(i) Reactive Dyes- Cibacron Brillant Red B, Procion Briilant Blue HB.

4. 1: Colour and Chemical Constitution of Dyes (5 L)

4.1.1: Absorption of visible light, colour of wavelength absorbed, Complementary colour.

4.1.2: Relation between colour and chemical constitution.

(i) Armstrong theory (quinonoid theory) and its limitations
(ii) Valence Bond theory; Comparative study and relation of colour in the following classes of compounds/dyes: Benzene, Nitrobenzene, Nitroanilines, Nitrophenols, Benzoquinones, Azo, Triphenyl methane, Anthraquinones.
(iii) Molecular Orbital Theory.

4.2: Non-Textile Uses of Dyes (6 L)

Structural features of the substrate, fastness and other property requirements and main classes of dyes used to be mentioned as applicable. (Two examples with structures for each of the following):

1. Leather
2. Paper
3. Foodstuff
4. Cosmetics
5. Medicinal
6. Biological Stains
7. Indicator & Analytical Reagents
8. Coloured Smokes & Camouflage colours , Laser Dyes

4.3: Optical Brighteners (2 L)

General idea and important characteristics of optical brighteners, one example each with structure of the following classes: Stilbene, Coumarin, Heterocyclic vinylene derivatives, Diaryl pyrazolines, Naphthalimide derivatives.

4.4: Organic Pigments (3 L)

General idea, distinguish between dyes and pigments, important characteristics of organic pigments, Toners, Lakes, Classification of organic pigments with suitable examples, i.e. Ionic pigments-Lake of acid and basic dyes. Nonionic pigments-Azo, Indigoid, Anthraquinone, Quinacridone, Phthalocyanine (Copper phthalocyanine).

REFERENCES

1. **Satoskar ,** Pharmacology and pharmaceutics Vol.I and II.
2. **Wilson and Gisvold** Textbook of organic, medicinal, and pharmaceutical chemistry.
3. **William O. Foye and David A. William,** Textbook of medicinal chemistry.
4. **G. R . Chatwal** Medicinal chemistry,
5. **K. Venkataraman** ,Chemistry of synthetic dyes, Vol. I to VI.
6. **H. A. Lubs ,**Chemistry of synthetic dyes and pigments.
7. **H. Zollinger,** Colour Chemistry.
8. **R. L. M. Allen,** Colour Chemistry.
9. **Groggins ,**Unit process.
10. **M. S. Yadav ,** Synthetic dyes.
11. **Thomas Vickerstaff,** Physical Chemistry of dyeing.
12. **V. A. Shenai**, Chemistry of dyes and principles of dyeing
13. **A. I. Vogel,** Practical Organic Chemistry,

CIA I: Short answer questions **20 MARKS**

CIA II: Short answer questions **20 MARKS**

Template of Question Paper

DRUGS AND COLOR CHEMISTRY **COURSE: S.CHE.5.AC**

OBJECTIVES

UNIT	KNOWLEDGE	UNDERSTANDING	APPLICATION	TOTAL MARKS
I	6	6	3	15
II	6	6	3	15
III	6	6	3	15
IV	6	6	3	15
TOTAL MARKS PER OBJECTIVES	24	24	12	60
% WEIGHTAGE	40	40	20	100

PRACTICAL CHEMISTRY **COURSE: S.CHE.5.AC.PR**

A. PREPARATIONS

1. Aspirin from Salicylic acid.
2. p-Nitroacetanilide from Acetanilide.
3. p-Nitroaniline from p-Nitroacetanilide.
4. m-Dinitrobenzene from Nitrobenzene
5. Fluorescein from Phthalic Anhydride
6. Anthraquinone from Anthracene

B. ESTIMATIONS

1. Estimation of Iodine in Tincture Iodine
2. Estimation of Ibuprofen

CIA : ESTIMATION OF DRUG/DYE **15 MARKS**

JOURNAL **5 Marks**

END SEMESTER PRACTICAL EXAMINATION **30 MARKS**

PREPARATION OF DRUG/DYE

The Practical Exam Will Be Conducted For 1 Session Of 3 Hours Duration.

BATCH SIZE FOR:

REGULAR PRACTICALS **20 STUDENTS PER IN-CHARGE**

EXAMINATIONS **MAXIMUM 20 STUDENTS PER BATCH**

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