ANDHRA UNIVERSITY

DEPARTMENT OF CHEMISTRY

PROGRAM : M.SC PHYSICAL CHEMISTRY
REGULATION AND SYLLABUS EFFECTIVE
FROM 2021-2022 BATCH

ANDHRA UNIVERSITY

SCHOOL OF CHEMISTRY

Revised Syllabus for M.Sc. PHYSICAL CHEMISTRY (PREVIOUS)

(With effect from the Admitted batch of 2021-2022 Academic Year)

Programme Objectives

1. To mould a generation of youth which can apply the subject knowledge in their life and careers
2. To inculcate scientific attitude enriched with a multidisciplinary perspective in the students.
3. To demonstrate broad knowledge of descriptive Chemistry.
4. To impart the basic analytical and technical skills to work effectively in the various fields of chemistry.
5. To motivate critical thinking and analysis skills to solve complex chemical problems, e.g., analysis of data, synthetic logic, spectroscopy, structure and modeling, team-based problem solving, etc.
6. To demonstrate an ability to conduct experiments in the above sub-disciplines with mastery of appropriate techniques and proficiency using core chemical instrumentation and modeling methods.
7. To demonstrate the ability to perform accurate quantitative measurements with an understanding of the theory and use of contemporary chemical instrumentation, interpret experimental results, perform calculations on these results and draw reasonable, accurate conclusions.
8. To demonstrate the ability to synthesize, separate and characterize compounds using published reactions, protocols, standard laboratory equipment, and modern instrumentation.

Programme Outcomes:

Students after completing M.Sc Analytical Chemistry course shall

PO1: Be able to demonstrate basic knowledge in the core areas of chemistry (analytical, general, inorganic, organic, physical, applied chemistry etc).

PO2: Have firm foundations in the fundamentals and application of current chemical and scientific theories in Inorganic, Organic, Physical and Analytical Chemistry.

PO3: Be versatile in classical laboratory techniques, use instrumental methods for analysis as well as synthesis and follow standardised procedures and regulations in handling and disposal of chemicals.

PO4: Become post graduates with the skills to critically assess and solve problems requiring the application of chemical principles.

PO5: Equip students with effective scientific communication skills

Programme Specific Outcomes of M.Sc Programme with Physical Chemistry

PSO1:- Provide theoretical background and develop practical skills for analysing materials using modern analytical methods and instruments

PSO2:- Inculcate a problem solving approach by coordinating the different branches of chemistry

PSO3:- Becomes professionally skilled for higher studies in research institutions and to work in chemical industries.

PSO4:- In-depth knowledge helps to qualify in competitive exams.

REGULATIONS

1. The duration of the course is for two academic years with total four semesters. The nature of the course is full-time.
2. Candidates for the degree of Master of Science in Chemistry shall be required to have passed the B.Sc. with Chemistry / Applied Chemistry / Industrial Chemistry as one the subject of this university or any other university recognized by the academic council as equivalent thereto.
3. The course and scope of instruction shall be as defined in the syllabus prescribed. (Annexure-III)
4. Candidate who takes instruction shall be required to take examinations at the end of each semester as specified in Annexure-I.
5. Each candidate has to undergo an internship for a duration of four weeks during the fourth semester in any chemical industry/ R&D / organization/ or at the department at their own expense and have to submit project report.
6. A candidate shall be declared to have passed in any course if he /she secures not less than "E" grade in theory and not less than "D" grade in the practical /Project, provided the result otherwise is withheld. There is no minimum pass marks for internal assessment marks both theory as well as practical.

A candidate shall be deemed to have satisfied the minimum requirement for the award of the degree of M.Sc. Chemistry.

i. If he / she is declared to have passed all the subjects included in the scheme of instruction and examination and
ii. if he /she secures 5.0 CGPA in each of the semesters by the end of the fourth semester.

Further, a candidate shall be permitted to choose any course(s) to appear for improvement in case the candidate fails to secure the minimum prescribed SGPA/CGPA to enable the candidate to pass at the end of any semester examinations. There shall not be any provision for the improvement of internal assessment marks in any theory or practical subjects in any year /semester of study. Grades and calculation of SGPA and CGPA are given in Annexure-II

7. The successful candidates in the M.Sc. Chemistry degree examination shall be arranged in the order in which they are registered for the examination in the following classes on the basis of the CGPA. However, students who pass in any supplementary examination shall not be awarded Distinction even if they obtain a CGPA of 8.0 or above, they shall be considered as First Class only.

First Class with Distinction	– CGPA 8.0 or more
First Class	– CGPA 7.0 or more but less than 8.0
Second Class/Pass	– CGPA 5.0 or more but less than 7.0

8. The Question course setting and valuation shall be as per the University regulations at the end of each semester.
9. The practical examinations shall be conducted and valued by both internal and external examiners at the end of each semester.
10. The viva- voce examination for Project Work shall be conducted both internal and external examiners at the end of the completion of project and after submission of the Project Report by each of the candidates.
11. The Minimum attendance required by a candidate will be 75% of the total number for

the working days in that semester. Provided that in special cases and for sufficient cause shown, the Vice-chancellor may, on the recommendation of the Principal and the Head of the department concerned, condone the deficiency in the average attendance to an extent of 9% for reasons such as ill health, if the application for condonation is submitted at the time of actual illness and is supported a certificate of an authorized medical officer approved by the Principal. However, 100% attendance should be maintained for all practicals/ labs/ Internship>

12. Each of the student has to study two MOOC courses from NPTEL/SWAYAM etc. one in the third semester and the other in the fourth semester of the programme and the grade obtained should be submitted to the Department/ College/ University for incorporation in the marks list along with the Grade/ Course Completion Certificate. The Departmental Committee shall decide whether to accept or not the grade/score obtained by the student. The student has to complete each of these courses during the concerned semester period only.
13. Keeping in view of the objectives of NPE 2020 and the directives of the University, two value added courses have been included each in 3rd and 4th semesters of the course. Intellectual Property rights in 3rd semester and Research Methodology in the 4th semester under non-credit scheme. However, the students have to attend the examination and pass the examination similar to that of other subjects of the course.
14. The University may, from time to time, revise, amend or change the regulations, scheme of examination and syllabus. In the case of students already undergoing the course, the changes will take effect from the beginning of the following academic year after the change are introduced and shall cover the part of the course that remains to be completed.

M.SC. CHEMISTRY WITH SPECIALIZATION PHYSICAL CHEMISTRY
SCHEME OF INSTRUCTION AND EXAMINATIO FOR I-SEMESTER

Course code	Course Title	Course type (Theory/ Practical)	Instruction periods per week	Internal Marks	External Marks	Total Marks	Duration of Examination	Credits
SC-C 117	General Chemistry-I	Theory	04	20	80	100	3 hrs	04
SC-C 118	Inorganic Chemistry-I	Theory	04	20	80	100	3 hrs	04
SC-C 119	Organic Chemistry-I	Theory	04	20	80	100	3 hrs	04
SC-C 120	Physical Chemistry-I	Theory	04	20	80	100	3 hrs	04
PR-347	Inorganic Chemistry Laboratory-1	Practical	06	15	60	75	3 hrs	03
PR-348	Physical Chemistry Laboratory-1	Practical	06	15	60	75	3 hrs	03
PR-349	Organic Chemistry Laboratory-1	Practical	06	15	60	75	3 hrs	03
		Total	34					25

M.SC. CHEMISTRY WITH SPECIALIZATION PHYSICAL CHEMISTRY
SCHEME OF INSTRUCTION AND EXAMINATIO FOR II-SEMESTER

Course code	Course Title	Course type (Theory/ Practical)	Instruction periods per week	Internal Marks	External Marks	Total Marks	Duration of Examination	Credits
SC-S 215	General Chemistry-II	Theory	04	20	80	100	3 hrs	04
SC-S 216	Inorganic Chemistry-II	Theory	04	20	80	100	3 hrs	04
SC-S 217	Organic Chemistry-II	Theory	04	20	80	100	3 hrs	04
SC-S 218	Physical Chemistry-II	Theory	04	20	80	100	3 hrs	04
PR-350	Inorganic Chemistry Laboratory-1I	Practical	06	15	60	75	3 hrs	03
PR-351	Physical Chemistry Laboratory-I1	Practical	06	15	60	75	3 hrs	03
PR-352	Organic Chemistry Laboratory-1I	Practical	06	15	60	75	3 hrs	03
		Total Number of credits						25

M.SC. CHEMISTRY WITH SPECIALIZATION PHYSICAL CHEMISTRY
SCHEME OF INSTRUCTION AND EXAMINATIO FOR III-SEMESTER

Course code	Paper	Course type (Theory/ Practical)	Instruction Periods Per Week	Internal Marks	External Marks	Total Marks	Duration of Examinatio n	Credits
SCP- S 310	Paper-I (Advanced Chemical Kinetics & Physical Chemistry of Polymers)	Theory	4	20	80	100	3hrs	04
SCP- S 311	Paper-II (Quantum Chemistry – II & Chemical Applications of Symmetry and Group Theory)	Theory	4	20	80	100	3hrs	04
SCP- S 312	Paper-III(Statistical Thermodynamics & Solution Equilibria of Proton-Ligand Complexes)	Theory	4	20	80	100	3hrs	04
SCP- S 315	Paper-IV (Instrumentation)	Theory	4	20	80	100	3hrs	04
(PR-866)	Practical -I (Chemical Kinetics)	Lab	3	20	80	100	6hrs	04
(PR-867)	Practical -II (Instrumentation)	Lab	3	20	80	100	6hrs	04
	MOOCs Course					-	-	02
						600		26

M.SC. CHEMISTRY WITH SPECIALIZATION PHYSICAL CHEMISTRY
SCHEME OF INSTRUCTION AND EXAMINATIO FOR IV-SEMESTER

Course code	Paper	Course type (Theory/ Practical)	Instruction Periods Per Week	Internal Marks	External Marks	Total Marks	Duration of Examination	Credits
SCP – S 412	Paper-I (Advanced Chemical Kinetics & Photo Chemistry)	Theory	04	20	80	100	3hrs	04
SCP – S 411	Paper-II(Quantum Chemistry –II & Numerical Methods for chemistry and Advanced Computer Programming)	Theory	04	20	80	100	3hrs	04
SCP – S 410	Paper-III(Advanced Thermodynamics and Solution Equilibria of Meal-Ligand Complexes)	Theory	04	20	80	100	3hrs	04
SMC-S 413	Paper-IV(Spectroscopy)	Theory	04	20	80	100	3hrs	04
(PR-868)	Practical -I (Chemical Kinetics)	Lab	03	80	80	100	6hrs	04
(PR-869)	Practical -II (Instrumentation)	Lab	03	80	80	100	6hrs	04
	Viva-Voce		-	-	-	50		02
	Project Work		-	-	-	100		04
	MOOCs Course					-		02
						750		32

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZATION
SEMESTER-I
PAPER-I: GENERAL CHEMISTRY-I
(With effect from the Admitted batch of 2021-2022 Academic Year)

Course Outcomes (COs)/Course Specific Outcomes (CSOs):

Upon completion of the course the students will be able to,

CO1: Learn and understand the selection rules and criteria for molecules to exhibit rotational and IRspectroscopy.

CO2: Understand the Classical and quantum mechanical theories of Raman spectroscopy and basic concepts of electronic spectroscopy.

CO3: Learn spectroscopic methods based on magnetic resonance principles.

CO4: Learn basics of group theory and its application in chemistry.

CO5: Understand the basic concepts of FORTRAN programming and its applications.

Learning Outcomes (LOs):

Upon completion of the course the student will be able

- To apply the spectroscopic methods for structure elucidation of molecules.
- To acquire knowledge of molecular symmetry and group theory and to solve chemical problems.
- To write FORTRAN programs for simple chemical problems.

COURSE CONTENT

UNIT – I

Rotational spectra of diatomic molecules-rigid rotor-selection rules-calculation of bond length-isotopic effect, second order stark effect and its applications, Infrared spectra of diatomic molecules-harmonic and anharmonic oscillators. Selection rules-overtones-combination bands calculation of force constant, anharmonicity constant and zero point energy. Fermi resonance, simultaneous vibration rotation spectra of diatomic molecules.

UNIT-II

Raman effect-classical and quantum mechanical explanations-Rotational Raman and vibrational Raman spectra, Electronic spectra of diatomic molecules-Vibrational coarse structure-intensity of spectral lines-Franck Condon principle-applications, Rotational fine structure-band head and band shading, Charge transfer spectra.

UNIT-III

Spin Resonance Spectroscopy: Principle and theory of NMR spectroscopy-Nature of spinning particle and its interaction with magnetic field. Chemical shift and its origin. Spin-Spin interaction-experimental methods. Application of NMR to structural elucidation-Structure of ethanol, dimethylformamide, styrene and acetophenone. Principle and theory of ESR-g-factor, hyperfine interactions-applications of ESR studies to the structure of free radicals, metal complexes.

UNIT-IV

Basic concepts of Symmetry and Group theory – Symmetry elements, symmetry operations and point groups – Schoenflies symbols – Classification of molecules into point groups – Axioms of Group theory – Group multiplication tables for C_{2V} and C_{3V} point groups – Similarity Transformation and classes – Representations – reducible and irreducible representations, Mulliken symbols, Orthogonality theorem and its implications, character table and its anatomy.

UNIT-V

Basic components of Computers, higher and lower level languages, Microsoft Fortran: constants, variables and operators, arithmetic expressions, assignment and replacement statements, Input and Output statements – Format free and Format directed I/O statements – Iw, Fw.d, Ew.d and Gw.d format specifications, conditional and unconditional statements – Logical IF, Block IF and Go To statements, Do statement – syntax and rules.

Application of Chemical Problems:

Flowcharts and Programs for

1. Statistical Analysis calculation of arithmetic mean, mean deviation, variance and standard deviation of replicate measurements.
2. Solution of Quadratic equation – calculation of the roots of a quadratic equation.
3. Calculation of the pH and hydrogen ion concentration of an aqueous solution of a strong acid taking into account the auto ionization of water.
4. Calculation of the root of a polynomial using Gauss-Newton method – Application to Vander-Waal's equation.
5. Calculation of the rate constant of a first order reaction or calculation of molar extinction coefficient using Beer-Lambert's Law by Linear least-squares method.

Text Books:

1. Symmetry and Spectroscopy of Molecules, K Veera Reddy, New Age International Publishers.
2. Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press.
3. Chemical Applications of Group Theory, F. A. Cotton Wiley Eastern Limited New Delhi.
4. Group Theory and its Applications to Chemistry, K. V. Raman, Tata McGraw – Hill Publishing Company Ltd., New Delhi.
5. Computer programming in Fortran-IV by V .Rajaraman, Prentice-Hall of India Pvt. Ltd., New Delhi.
6. Molecular Spectroscopy, - Gordon M. barrow
7. Fundamentals of Molecular Spectroscopy – Banwell.

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECIALIZATION
SEMESTER-I
PAPER-II: INORGANIC CHEMISTRY-I
(With effect from the admitted batch of 2021-2022 academic year)

Course Objectives: To make the students

CO1: Acquiretheknowledgeon applications of VSEPR, Valence Bond and Molecular orbital theories in explaining thestructures of simple molecules **and** role of p and d orbitals in pi bonding.

CO2: Understandthe concept of MO theory to square planar ($PtCl_4^{2-}$) and Octahedral complexes (CoF_6^{3-}, $Co(NH_3)_6^{3+}$).And Walsh diagram for H_2O molecule

CO3: Apply theknowledgeandunderstandingofUnderstand the Orgel and Tanabe-Sugano diagrams for d^1 –d^9 octahedral and tetrahedral transition metal complexes of 3d series tonewly prepared metal complexes

CO4: Develop interest in the areas of magnetic properties of transition and inner transition metal complexes – spin and orbital moments – quenching of orbital momentum by crystal fields in complexes.

CO5: To understand the concept of Term symbols and Electronic spectra and Magnetic properties of complexes

LearningOutcomes: Attheendofthecourse,thelearnersshouldbeableto:

LO1: Explainidea of structure and bonding theories of inorganic compounds

LO2: InterpretWalsh diagram for other liner and bent molecules

LO3: Introduce electron counting rules for higher boranes

LO4: Analyse the preparation and structures of heteropoly acids

LO5: Understanding structure and bonding in coordination compounds

LO6: Explain selections rules, Tanabe-Sugano diagrams. Orgel diagrams

LO7: Experimentally Identify the covalency in metal complexes.

LO8: To calculate the magnetic susceptibility of metal complexes

LO9: Understand and analyse structure-property correlation of coordination compounds

LO10: Design new coordination compounds based on a fundamental understanding of their electronic properties

COURSE CONTENT

UNIT-1

Structure & Bonding: Applications of VSEPR, Valence Bond and Molecular orbital theories in explaining the structures of simple molecules- role of p and d orbitals in pπ-dπ bonding, Bent's rule, Non-valence cohesive forces

Application of MO theory to square planar ($PtCl_4^{2-}$) and Octahedral complexes (CoF_6^{3-}, $Co(NH_3)_6^{3+}$). Walsh diagrams for linear (BeH_2) and bent (H_2O) molecules

UNIT-II

Inorganic cage and ring compounds – preparation, structure and reactions of boranes, carboranes, metallocarboranes, boron–nitrogen ($H_3B_3N_3H_3$), phosphorus–nitrogen ($N_3P_3Cl_6$) and sulphur-nitrogen (S_4N_4, $(SN)_x$) cyclic compounds. Structure and bonding in higher boranes with (special reference to B12 icosahedra). Electron counting rules in boranes – Wades rules (Polyhedral skeletal electron pair theory).

Polyacids: Introduction to polyacids- Types of polyacids- Isopolyacdis, Isopoly molybdates, Isopolytungstates, Isopolyvanadates, Structures of Polyacids $]Mo_7O_{24}],^{6-}(V_{10}O_{28})^{6-}$ and $W4O_{16}]^{8-}$, Heteropolyacids- properties of heteropolyacids and salts, structures of heteropolyacids and theories , Mialalicopause and Roscnneium theories , Pauling's theory and keggin's theory, applications of polyacids.

UNIT-III

Coordination compounds: Crystal field theory - crystal field splitting patterns in octahedral, tetrahedral, tetragonal, square planar, square pyramidal and trigonal bipyramidal geometries. Calculation of crystal field stabilization energies. Factors affecting crystal field splitting energies – Spectrochemical series, Jahn – Teller theorem (static and dynamic Jahn-Teller theorem) and its consequences, nephelauxetic effect, applications and limitations of CFT; ligand field theory

Experimental evidences for covalence in complexes. Molecular Orbital Theory of bonding for Octahedral, tetrahedral and square planar complexes. π-bonding and MOT - Effect of π - donor and π -acceptor ligands on Δo. Experimental evidence for π - bonding in complexes

UNIT- IV

Electronic spectra of transition metal complexes:

Term symbol-Free Ion terms and Energy Levels: Configurations, Terms, States and Microstates, calculation of Microstates for P^2 and d^2 Configuration, Russell- Saunders Coupling Schemes, J-J Coupling scheme, derivation of terms for various configurations P^2 and d^2 configuration, spectroscopic Ground state , Hole Formalism, Energy ordering of terms (Hund's Rules), Selection rules: Laporte orbital selection rule, spin selection rules. Splitting of energy levels and spectroscopic states Orgel diagrams of d^1 to d^9 metal complexes. Interpretation of electronic spectra of aquo Complexes of Ti(III), V(III), Cr(III), Mn(II), Fe(II), Fe(III), Co(II), Ni(II) and Cu(II). Calculation of interelectronic and spectral parameters for d^8 metal complexes.

UNIT- V

Tanabe- Sugano diagrams for d^1 –d^9 octahedral and tetrahedral transition metal complexes of 3d series. Calculation of Dq, Racah Parameter (B) and nephelauxetic parameter (β), Charge transfer (L→M and M→L) spectra of metal complexes.

Magnetic properties of metal Complexes: Types of magnetic behavior, Temperature independent paramagnetism. Magnetic properties of transition and inner transition metal complexes – spin and orbital moments – quenching of orbital momentum by crystal fields in complexes. Magnetic susceptibility and its determination by Gouy's method, and Faraday's method. orbital contribution to magnetic moment ($O_h$and T_d Complexes)

Text books:

1. Advanced Inorganic Chemistry by F.A. Cotton and G. Wilkinson, IV Edition, John Wiley and Sons, New York, 1980.
2. Inorganic Chemistry by J.E. Huheey, III Edition, Harper International Edition, 1983.
3. Theoretical Inorganic Chemistry, II Edition by M.C. Day and J. Selbin, Affiliated East-West press Pvt. Ltd., New Delhi.
4. Inorganic Chemistry by Shriver and Atkins, Oxford University Press (1999)

ANDHRA UNIVERSITY

SCHOOL OF CHEMISTRY

REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECIALIZATION

SEMESTER-I

PAPER-III: ORGANIC CHEMISTRY-I

(With effect from the admitted batch of 2021-2022 academic year)

Course Objectives: To make the students

CO1: Acquiretheknowledgeofaliphaticnucleophilic,aliphaticelectrophilic,stereochemistryand conformational analysis, chemistry of heterocyclic compoundsandchemistryofnaturalproducts

CO2: Understandaliphaticnucleophilic, aliphaticelectrophilic, stereochemistry andconformational analysis, chemistry of heterocycliccompounds and chemistry ofnaturalproducts

CO3: Apply theknowledgeandunderstandingofaliphaticnucleophilic,aliphaticelectrophilic, stereochemistry and conformational analysis, chemistry of heterocyclic compounds and chemistry of natural products to new situations

CO4: Develop interest in the areas of aliphatic nucleophilic, aliphatic electrophilic,stereochemistry and conformational analysis, chemistry of heterocyclic compoundsandchemistryofnaturalproducts

LearningOutcomes: Attheendofthecourse,thelearnersshouldbeableto:

LO1: Explainaliphaticnucleophilic,aliphatic electrophilic,stereochemistryandconformational analysis, chemistry of heterocycliccompounds and chemistry ofnaturalproducts

LO2: Interpretaliphaticnucleophilic,aliphatic electrophilic,stereochemistryandconformational analysis, chemistry of heterocycliccompounds and chemistry ofnaturalproducts

LO3: Comparealiphaticnucleophilic, aliphaticelectrophilic,stereochemistryandconformational analysis, chemistry of heterocycliccompounds and chemistry ofnaturalproducts

LO4: Analysealiphaticnucleophilic,aliphaticelectrophilic,stereochemistryandconformationalanalysis, chemistry of heterocycliccompounds and chemistry ofnaturalproducts

LO5: Solvealiphaticnucleophillic,aliphaticelectrophilic,stereochemistryandconformational analysis, chemistry of heterocycliccompounds and chemistry ofnaturalproducts

LO6: Identify aliphatic nucleophilic,aliphaticelectrophilic, stereochemistry andconformationalanalysis,chemistryofheterocycliccompoundsand chemistryofnaturalproducts

LO7: Apply aliphaticnucleophilic,aliphaticelectrophilic, stereochemistry andconformationalanalysis,chemistryofheterocycliccompoundsand chemistryofnaturalproducts

COURSE CONTENT

UNIT–I

Aliphatic Nucleophilic Substitutions: The SN2, SN1, SNi and SET mechanisms.Substitutionreactionsofambidentnucleophiles,anchimericassistance,theneighbouring group mechanism: neighbouring group participation by 0,N, S,halogens, aryl groups, alkyl and cycloalkyl groups in nucleophilic substitutionreactions. Sigma, Pi bond participation in acylic and bicyclic systems (Non-classiccarbocations).NucleophilicSubstitutional allylic,ŁrigonalandVinyliccarbons.Effectofsubstrate,attackingnucleophile,leavinggroupandreactionmedium

UNIT-II

Aliphatic Electrophilic Substitutions: SEI SE2 and SEi mechanisms. Reactivity-effects of substrate, leaving group and solvent. Reactions- hydrogen exchange,migration of doublebonds, halogenation of aldehydes, ketones, carboxylic acids, acylhalides,sulphoxidesandsulphones.

UNIT-III

Stereochemistry and Conformational Analysis: Optical Isomerism:FiCal activity,moleculardissymmetryand chirality- elements of symmetry.Fisher'sprojectionD,L. and R,S. configurations - relative and absolute configurations optical isomerismdue to asymmetric carbon atoms - optical isomerism in biphenyls, allenes andspirans-opticalisomerismofnitrogenouscompounds,racemisationandresolution.

Geometricalisomerism:E,Z-configurations,propertiesofgeometricalisomers.Conformationalanalysis:Conformationsofacyclicmolecules-alkanesandsubstitutedalkanes-compoundshavingintramolecularhydrogenbonding.Conformations of cyclohexane, mono and disubstituted cyclohexanes and decalins,effectofconformationsonreactivity.

UNIT—IV

Chemistry of Heterocyclic Compounds :Structure, reactivity and synthesis of threemembered Heterocycles: (a) Oxirane: Sharpless method, Shi epoxidation, Jacobsenepoxidation, etc, (b) Aziridine; four membered Heterocycles: (a) Oxetane (b) Azetine;five memberedHeterocycles:(a) Pyrrole: Paa1 Knorr, Hantzsch Methods,etc, (b)Thiophene: Paa1 Knorr, Hinsberg method, etc. (c) Furan: Paa1 Knorr, Fiest-Benary,IndustrialMethod, etc.; (d) Pyrazole,(e) Imidazole,(f) Oxazole, (g) Thiazole; Sixmembered Heterocycles: (a) Pyridine, (b)Pyridazine,(c) pyrimidine and (d) Pyrazine;Aromatic heterocyclics: a) Indole: Fischer indole synthesis, Bischler synthesis, andMadelungsynthesis(b)QuinolineandIsoquinoline,(c)CoumarinsandChromones.

UNIT—V

Chemistry of Natural Products:

Terpenoids:-Occurrence,Isolation,isoprenerule,structureelucidationandsynthesisofn-Terpineolandn-pinene

Steroids:-Nomenclatureofsteroids,structureelucidation,synthesisandstereochemistryofcholesterolandprogesterone

Lipids:-Classification,propertiesandfunction-freefattyacids,triglycerides,phospholipids,glycolipids&waxesconjugatedlipids-lipoproteins

.**ReferenceBooks**

1. AdvancedOrganicChemistry:ReactionsMechanismsandStructurebyJerryMarch, Mc.GrawHillandKogakush.

2. OrganicChemistryVol.I(Sixth Ed.)andVol.II(FifthEd.)byILFinarELBS.

3. OrganicChemistry(fifthEd.,)byMorrison andBoyd,PHI,India.

4. OrganicChemistry(fifthedition)byFrancisA.CareyTataMcGrawHillpublishing CompanyLimited,NewDelhi.

5. StereochemistryofOrganiccompoundsbyErnestL.E1ie1,SamuelH.Wilen

6. Chemistry of natural products by S. V. Bhat, B. A. Nagasampangi and M.Sivakumar NarosaPublishingHouse,6threprint2010

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECIALIZATION
(With effect from the admitted batch of 2021-2022 academic year)
SEMESTER-I
PAPER-IV: PHYSICALCHEMISTRY-I
(With effect from the admitted batch of 2021-2022 academic year)

Course Outcomes (COs)/Course Specific Outcomes (CSOs)
Upon completion of the course the students will be able to,

CO1: Explain the basic concepts of Thermodynamics and its applications

CO2: Understand the concepts of thermodynamics of solutions.

CO3: To understand the principle of micellisation.

CO4: Understand the various kinetic theories, measurements of reaction rates.

CO5: Learn experimental techniques for measuring the kinetics of fast reactions and homogenous catalyzed reactions.

Learning Outcomes (LOs):
Upon completion of the course the student will be able to understand

LO1: To apply the concepts of thermodynamics to various problems in chemistry.

LO2: To predict various reaction mechanisms.

LO3: To apply the concept of micellization to various chemical reactions.

COURSE CONTENT

UNIT-I

Basic concepts of second law of Thermodynamics-Entropy- Entropy changes accompanying different processes-Entropy changes in an ideal gas, entropy changes in the mixing of ideal gases, entropy as a function of V and T and entropy as a function of P and T- Entropy change in isolated systems- Clausius inequality-Helmholtz and Gibbs energy -Maxwell relations - Criteria for spontaneity-variation of Gibbs energy with temperature and pressure for solids, liquids and gases-Concept of fugacity-determination of fugacity coefficient of gases- Thermodynamics of phase transitions- Concept of chemical potential-Location of phase boundaries- (Clausius-Clapeyron equation for Liquid- Vapour, Solid -Liquid and Solid- Vapour boundaries)- Ehrenfest classification of phases.

UNIT-II

Thermodynamics of mixtures -partial molar quantities - experimental methods of determination of partial molar quantities -Gibbs-Duhem equation and Duhem-Margules equation-Thermodynamics of mixing of liquids (ΔH_{mix}, ΔG_{mix} and ΔS_{mix}) - Thermodynamics of ideal solutions - Raoult's law -Thermodynamics of colligative properties of dilute solutions - concept of activity and activity coefficient-Experimentaldetermination of activity coefficient - Thermodynamic concept of equilibrium, variation of equilibrium with temperature (Van't Hoff equation) and pressure - Nernst heat theorem, Third law of thermodynamics- exceptions to third law of thermodynamics.

UNIT-III

Surface tension- Capillary action- Adsorption-Adsorption isotherms- Freundlich adsorption isotherm, Langmuir adsorption isotherm-limitations - BET adsorption isotherm-estimation of Surface area.Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization- phase separation and mass action models.

UNIT-IV

Chemical Kinetics: Theories of reaction rates- Collision theory- Limitations, Transition state theory.Lindeman's theory of unimolecular reactions -Limitations. Diffusion controlled reactions. Effect of ionic strength on rates of reactions- Primary and secondary salt effects. Effect of dielectric constant onreactions - kinetic isotope effect -Primary and secondary isotopic effects -Effect of substituent -Linear free energy relationships - Hamett equation - limitations- Taft equation. Kinetics of consecutive reactions, parallel reactions, opposing reactions (Uni molecular steps only, no derivation).

UNIT-V

Specific and general acid-base catalysis. Skrabal diagrams. Steady state approximation- Enzyme catalysis- Michaelis -Menten mechanism. Derivation of Kinetic equation and Kinetic parameters. Lock and Key hypothesis-pH dependence of enzyme catalyzed reactions.Fast reactions- different methods of studying fast reactions- flow methods, relaxation methods- temperature jump and pressure jump methods.

Text Books:

1. Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press.
2. Chemical Kinetics by K. J. Laidler, McGraw Hill Pub.
3. Physical chemistry by K.L. Kapoor

Reference Books:

1. Thermodynamics for Chemists, Samuel Glasstone
2. Physical chemistry by Puri, Sharma and Pathania
3. Micelles, Theoretical and applied aspects, V. Moroi, Plenum publisher

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECIALIZATION
SEMESTER-I
PRACTICAL-I: INORGANICCHEMISTRY
(With effect from the admitted batch of 2021-2022 academic year)

Course Objectives:

CO1: To develop an insight into the preparation of inorganic complexes
CO2: To understand the process of preparation of inorganic complexes
CO3: To acquire skills in the preparation of inorganic complexes

Learning Outcomes:

At the end of the course, the learners should be able to:

LO1: Prepare various inorganic complexes
LO2: Develop skill in handling apparatus, measure the quantities and carryout the reaction and analyse the inorganic mixtures
LO3: Applies the skill in preparing new metal complexes and analysis of inorganic mixtures
LO4: Understand the regulations in handling and disposal of chemicals.

COURSE CONTENT:

1. **Synthesis of Inorganic Metal Complexes:**Synthesis of 3d transition metal complexes of tetrahedral, square planar and octahedral geometries.
   (i) Preparation of TetraammineCopper(II) sulphate monohydrate
   (ii) Potassium tris-oxalatoferrate (III) trihydrate
   (iii) Tris-thiourea copper(I) sulphate

2. **Systematic SemimicroQualitative Analysisof Inorganicsix radical mixtures**
   In systematic Semi micro qualitative inorganic analysis, inorganic mixture containsthree cations and three anions. The analysis involves identification and conformation of cations and anions containing one less familiar cation(Tungsten, Molybdenum, Zirconium, Thorium, Titanium, Uranium, Cerium, Vanadium, Lithium, Berkelium Etc... and one interfering anion

Anions: CO_3^{2-}, S^{2-}, SO_3^{2-}, Cl^-, Br^-, I^-, NO_3^-, SO_4^{2-}, CH_3COO^-, $C_2O_4^{2-}$, $C_4H_4O_6^{2-}$, PO_4^{3-}, CrO_4^{2-}, AsO_4^{3-}, F^-, BO_3^{3-}

Cations : Ammonium (NH_4^+),1st group: Hg, Ag, Pb, Tl, W ; 2nd group: Hg, Pb, Bi, Cu, Cd, As, Sb, Sn, Mo; 3rd group: Fe, Al, Cr, Ce, Th, Ti, Zr, V, U, Be
4th group: Zn, Mn, Co, Ni5th group: Ca, Ba, Sr6th group: Mg,K, Li

Note: A minimum of 4 inorganic mixtures must be analysed in this Semester

REFERENCE BOOKS:

1. Practical Inorganic Chemistry, G. Marr and B. W. Rockett.

2. Practical Inorganic Chemistry by G.Pass H.Sutchiffe,2nd edn John Wiley & Sons.

3. Experimental Inorganic/Physical Chemistry, M. A. Malati, Horwood Publishing, Chichester, UK (1999)

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SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECIALIZATION
SEMESTER-I
PRACTICAL-II: PHYSICALCHEMISTRY
(With effect from the admitted batch of 2021-2022 academic year)

Course Objectives:

CO1: To maintain laboratory ethics, safety and cleanliness
CO2: To Preparation and standardization of solutions
CO3: To have hands-on experience/practical knowledge in performing Physical chemistry experiments
CO4: To develop skills on handling instruments like conductometry and perform different types of acid-base titrations
CO5: To plot accurate graphs of the desired scale for the calculations of Langmuir and Freundlich isotherms
CO6: To Prepare the solution of the desired concentration and the desired volume in Cuprammonium cation.

LearningOutcomes:

At the end of the course, the learners should be able to:

LO1: To be able to develop/practical skills to solve problems in chemistry.
LO2: To extend the principle of Conductometric titration to other kind of reactions.
LO3: To learn to use the concept of phase diagram for different systems
LO4: To apply adsorption isotherms for other reactions.

COURSE CONTENT:

1. Conductometry
   a) Conductometric titration of strong acid (HCl) vs strong base (NaOH)
   b) Conductometric titration of weak acid (CH_3COOH) vs strong base (NaOH)
   c) Conductometric titration of mixture of acids (HCl + CH_3COOH) vs strong base (NaOH)
2. Determination of Cell constant of conductivity cell
3. Determination of Dissociation constant of weak acid by conductometric Method
4. Determination of Critical solution temperature of phenol-Water system
5. Determination of effect of electrolyte (NaCl) on the miscibility temperature of Phenol-Water system
6. Determination of composition of Cuprammonium cation using partition coefficient method
7. To verify Langmuir and Freundlich isotherm for absorption of acetic acid onto activated Charcoal

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SEMESTER-I
PRACTICAL-III: ORGANICCHEMISTRY
(With effect from the admitted batch of 2021-2022 academic year)

Course Objectives:

CO1: To develop an insight into the preparation of organic compounds in various reactions

CO2: To understand the process of preparation of organic through various reactions

CO3: To acquire skills in the preparation of organic compounds, their separation, purification and identification

Learning Outcomes:

At the end of the course, the learners should be able to:

LO1: Prepare various organic compounds using various reactions

LO2: Develop skill in handling apparatus, measure the quantities and carryout the reaction, separate the products, purify them and analyse the products formed

LO3: Applies the skill in preparing novel organic moieties

COURSE CONTENT:

Synthesis of Organic compounds

Synthesis, purification and characterization of about ten organic compounds involving one or two stages.

List of some suggested compounds

1. β-Napthyl methyl ether from β-Naphthol
2. m-dinitrobenzene from Nitrobenzene
3. Azo dye from primary amine
4. Aromatic acid from ester
5. Benzanilide from aniline
6. p-nitroaniline from Acetanilide
7. p-Bromo acetanilide from aniline
8. Phthalimide from phthalic acid
9. 1,2,3-Tribromo benzene from aniline
10. Benzanilide from Benzophenone

Text Books:

1. A Textbook of Practical Organic Chemistry by A. I. Vogel, ELBS and Longman group.
2. Practical Organic Chemistry by Mann and Saunders, ELBS and Longman group

MODEL QUESTION PAPER
ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECIALIZATION
SEMESTER-I
Paper- I: GENERAL CHEMISTRY-I
(With effect from the admitted batch of 2021-2022 academic year)

Time: 3 Hours **Max. marks: 80 (5X16 =80 marks)**

Answer ALL questions

1. (a) (i) What kind of molecules exhibit microwave spectra.
   (ii) Discuss isotope effect in microwave spectra.
   (or)
   (b) (i) Derive an expression for energy or harmonic oscillator and discuss the selection rules.
   (ii) Describe the origin of PQR structure of Vibrational-Rotational spectra.

2. (a) (i) Discuss the classical and quantum mechanical theories of Raman spectra
   (ii) Explain rotational fine structure in electronic spectroscopy?
   (or)
   (b) (i) State and explain Franck Condon principle.
   (ii) Write a short note on charge transfer spectra.

3. (a) (i) Explain the terms spin active nuclei, resonance, Larmor precession and chemical shifts in NMR.
   (ii) Explain hyperfine interactions in ESR spectroscopy taking examples.
   (or)
   (b) (i) What are the factors affecting ‘g’ value in ESR spectroscopy.
   (ii) Explain spin-spin interactions in NMR spectroscopy?

4. (a) (i) State and explain the axioms of group theory.
   (ii) State the great Orthogonality theorem and discuss its implications
   (or)
   (b) (i) Give the points groups for NH_3, XeF_4, eclipsed C_2H_6, Cis C_2H_4, B_3,N_3H_6 and allene
   (ii) Describe the anatomy of character table.

5. (a) (i) Write a flowchart and FORTRAN program for calculation of rate constant of a first order reaction.
   (ii) Give the syntax and rules of DO statement
   (or)
   (b) (i) Write a flowchart and FORTRAN program for calculation of pH and hydrogen ion concentration of an aqueous solution of a strong acid taking into account the auto ionization of water
   (ii) Write a brief note on format direction Input/output statements.

MODEL QUESTION PAPER
ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECIALIZATION
SEMESTER-I
Paper- II: INORGANIC CHEMISTRY-I
(With effect from the admitted batch of 2021-2022 academic year)

Time: 3 Hours **Max. marks: 80 (5X16 =80 marks)**

Answer ALL questions

1. (a) (i) Predict the geometries of ClF_3, XeF_4 and SF_4 molecules using VSEPR theory
   (ii) What is LCAO method? Predict bond order and bond lengths in O_2^+ and O_2^- ions based on MO energy level diagram
   (or)
   (b) (i) Draw the MO energy level diagram for $[Co(NH_3)_6]^{3+}$ and discuss its magnetic properties
   (ii) Draw the Walsh diagram for H_2O molecule and predict its structure.
2. (a) (i) Discuss the preparation of, structure of, and bonding in $N_3P_3Cl_6$.
   (ii) Discuss the structure and properties of borazole
   (or)
   (b) (i) Explain Mialalicopause and Rosenneium theories Pauling's theory and Keggin's theory of polyacids.
   (ii) Explain the method of counting skeletal electrons in cluster compounds
   (or)
3. (a) (i) Draw and explain the crystal field splitting of 'd' orbitals in square planar and trigonal bipyramidal geometries.
   (ii) Discuss the factors affecting crystal field splitting energies.
   (or)
   (b) (i) What are static and dynamic Jahn-Teller theorem and discuss its consequences
   (ii) Write a note on nephelauxetic effect
4. (a) (i) How do Tanable-Sugano diagrams differ from Orgel diagram? Draw Tanabe-Sugano diagram for $[V(H_2O)_6]^{3+}$
   (ii) Draw the Orgel diagram for $[TiCl_4]^-$ ion and explain the electronic transition
   (or)
   (b) (i) Write an account on Russell – Saunders coupling.
   (ii) Derive the terms symbols for Ni^{2+} and identify the ground state term symbol
5. (a) (i) Discuss different types of paramagnetic behaviour of transition metal complexes
   (ii) Calculate the spin only magnetic moments of the $[MnCl_6]^{3-}$ and $[Fe(CN)_6]^3$
   (or)
   (b) (i) Describe the Magnetic properties of inner transition metal complexes
   (ii) Determination of magnetic susceptibility a determination by Gouy's and Faraday's methods

MODEL QUESTION PAPER
ANDHRA UNIVERSITY
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REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECIALIZATION
SEMESTER-I
Paper- III: ORGANIC CHEMISTRY-I
(With effect from the admitted batch of 2021-2022 academic year)

Time: 3 Hours **Max. marks: 80 (5X16 =80 marks)**

Answer ALL questions

1. (a) (i) Explain SN_2 reaction with stereo chemical evidence
   (ii) What are non-classical carbocations? Explain them.
   (or)
   (b) (i) Describe neighbouring group participation reactions of Oxygen and Halogens with an examples.
   (ii) Write a note on nucleophilic substitution reaction at allylic and trigonal carbons

2. (a) (i) Explain SE1 and SE2 reactions with examples.
   (ii) Write a note on halogenations of ketones and carboxylic acids with examples
   (or)
   (b) (i) Write a note on SE^i reaction and migration of double bonds
   (ii) Describe halogenations of sulphoxide and sulphones

3. (a) (i) Explain optical isomerism of biphenyls and spirans
   (ii) Write about racemization and resolution with examples
   (or)
   (b) (i) Describe the properties of geometrical isomers.
   (ii) Write the conformational analysis of cyclohexane with an example

4. (a) (i) Write any two synthesis and reactivity of Oxirane
   (ii) Explain any two synthesis and reactivity of Indole
   (or)
   (b) (i) Describe the synthesis and properties of Pyridine
   (ii) Write a note on coumarins and chromones with examples

5. (a) (i) Explain the synthesis of *a*-pinene
   (ii) Write any synthesis of progesterone
   (or)
   (b) (i) Explain triglycerides with examples
   (ii) Write the structure elucidation of cholesterol

MODEL QUESTION PAPER
ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECIALIZATION
SEMESTER-I
Paper- IV: PHYSICAL CHEMISTRY-I
(With effect from the admitted batch of 2021-2022 academic year)

Time: 3 Hours **Max. marks: 80 (5X16 =80 marks)**

Answer ALL questions

1. (a) (i) Derive Maxwell's relations
   (ii) Define fugacity. How do you determine the fugacity of real gases?
   (or)
   (b) (i) Derive Clausius-Clapeyron equation
   (ii) Explain the entropy changes accompanying in different processes

2. (a) (i) Define partial molar quantity? Explain the experimental methods for determining partial molar quantities.
   (ii) Explain briefly about thermodynamics of mixing of liquids
   (or)
   (b) (i) State and explain third law of thermodynamics and write its limitations
   (ii) What is effect of temperature on equilibrium constant?

3. (a) (i) Discuss the features and limitations of Langmuir adsorption isotherm
   (ii) Give a classification of surface-active agents along with examples
   (or)
   (b) (i) What are important features of BET isotherm
   (ii) What is CMC? What are the factors affecting CMC

4. (a) (i) Discuss the Lindeman theory of unimolecular reaction and its limitations
   (ii) Write a note on diffusion-controlled reactions
   (or)
   (b) (i) Derive an expression for effect of ionic strength on rate of reaction
   (ii) Discuss the kinetics of consecutive reactions

5. (a) (i) Explain the Michaelis-Menten mechanism for enzyme catalysis
   (ii) Explain the mechanism of specific acid-base catalysis
   (or)
   (b) (i) Explain steady-state approximation with examples
   (ii) Explain temperature jump method for fast reactions and derive an expression for relaxation time

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SEMESTER-II

PAPER-I: GENERAL CHEMISTRY-II

(With effect from the admitted batch of 2021-2022 academic year)

Course Objectives:

CO1 Students will have the idea of wave function and understand the uncertainty relations

CO2 Students will learn how to solve the Schrodinger Eq. rigorously for model systems

CO3 Students will be able to understand and be able to explain the origin of quantized energy levels

CO4 Students will learn to apply concepts from physics and methods from mathematics to derive and understand the properties of chemical systems that arise from quantum mechanical models for the structure of atoms and molecules

CO5 They will be able to understand and explain the differences between classical and quantum mechanics

Learning Outcomes:

LO1 Gain knowledge about wave equation-interpretation of wave function-properties of wave function-normalization and orthogonalization.

LO2 Understand about symmetry arguments in deriving the selection rules, the concepts of tunneling-particle in three-dimensional box. Calculations using wave functions of the particle in a box.

LO3 Gain knowledge about Perturbation theory-time independent perturbation (only first order perturbation is to be dealt with) – application to ground state energy of helium atom

LO4 Study about variation principle-applications-calculation of zero-point energy of harmonic oscillator-many electron atom

LO5 Gain knowledge about Valence bond approach-directed valence-hybridization-covalent bond-calculation of ionic and covalent bond contributions in hydrogen molecule

LO6 Gain knowledge about hydrogen molecule ion-hydrogen molecule (fundamental concepts only

COURSE CONTENT

Unit I

Wave equation – interpretation of wave function – properties of wave function – normalization and orthogonalisation, operators – linear and non-linear commutators of operators, Postulates of quantum mechanics, setting up of operators observables – Hermitian operator – Eigen values of Hermitian operator.

Unit-II

Wave mechanics of simple systems with constant potential energy, particle in one dimensional box – factors influencing colour – transition – dipole integral, symmetry arguments in deriving the selection rules-the concept of tunneling – particle in a three dimensional box, Rigid rotor, wave mechanics of systems with variable potential energy-simple harmonic oscillator-solution of wave equation-selection rules.

UNIT-III

Hydrogen atom-solution of R(r), $\theta(\theta)$ and $\Phi(\phi)$ equations-probability density in orbitals-shapes of orbitals. Perturbation theory-time independent perturbation (only first order perturbation is to be dealt with) – application to ground state energy of hydrogen and helium atom

UNIT –IV

Variation principle-applications to hydrogen and helium atoms-calculation of zeropoint energy of harmonic oscillator-many electron atom- Comparison between Perturbation and variation theorems. Hartee-Fock self-consistent field method and introductory concepts of Density functional theory(DFT).

UNIT-V

Valence bond approach-directed valence-hybridization-covalent bond-calculation of ionic and covalent bond contributions in hydrogen molecule. Molecular orbital theory – LCAO approximation – hydrogen molecule ion – hydrogen molecule (fundamental concepts only) – The electronic transitions in the hydrogen molecule.

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SEMESTER-II
PAPER-II: INORGANICCHEMISTRY-II
(With effect from the admitted batch of 2021-2022 academic year)

Course Objectives: To make the students

CO1 To give a basic and updated knowledge for the students on metal clusters, Organometallic chemistry of transition metals

CO2 To discuss the preparation and structures of and functional aspects of metal clusters

CO3 Design new coordination compounds based on a fundamental understanding of their electronic properties

CO4 To discuss basics principles of reaction mechanism in metal complexes

CO5 To understand the concept of Term symbols and Electronic spectra and Magnetic properties of complexes

LearningOutcomes: Attheendofthecourse,thelearnersshouldbeable to:

LO1 Explain the idea of metal clusters

LO2 Interpret the bonding nature in metal clusters

LO3 Understand the basics of inorganic and coordination chemistry

LO4 Verity the 18 electron rules in various metal clusters

LO5 Determine the stability constants of metal complexes

LO6 Explain the kinetics of substitution reaction, conjugate bas mechanism and trans effect

LO7 Design new coordination compounds based on a fundamental understanding of their Reaction mechanism

COURSE CONTENT

UNIT-I

Metal cluster compounds - definition – evidences for existence of M-M bonds - conditions favorable for formation of M-M bonds – preparation, structure and bonding of the following metal cluster compounds.

$Re_2Cl_8^{2-}$, $Mo_2Cl_8^{4-}$, $Re_2(RCOO)_4X_2$, $Mo_2(RCOO)_4(H_2O)_2$, $Cr_2(RCOO)_4(H_2O)_2$, $Cu_2(RCOO)_4(H_2O)_2$, $Cr_2Cl_9^{3-}$, $Mo_2Cl_9^{3-}$, $W_2Cl_9^{3-}$, Re_3Cl_9, $Re_3Cl_{12}^{3-}$, $Mo_6Cl_8^{4+}$, $Nb_6X_{12}^{2+}$ and $Ta_6X_{12}^{2+}$.Polyatomic clusters – Zintle ions, Chevrel phases.

UNIT-II

Organometallic compounds - 16 and 18 electron rules.
Isoelectronicrelationship - Synthesis, structure, bonding and reactions of carbon monoxide, dinitrogen and nitric oxide complexes.
Isolobal relationship – H, Cl, CH_3, $Mn(CO)_5$; S, CH_2, $Fe(CO)_4$; P, CH, $Co(CO)_3$
Synthesis, structure, bonding and reactions of metallocenes with special reference to ferrocene

UNIT-III

Metal Ligand equilibria in solution:
Step wise and overall formation constants and their interaction. Trends in stepwise constants ((statistical effect and statistical ratio), factors affecting the stability of metal complexes; Stability correlations - Irwing -William's series, Pearson's theory of hard and soft acids and bases (HSAB), Application of HSAB: Biological functions and toxicology of metals, and medicinal applications; chelate effect and its thermodynamic origin

UNIT-IV

Determination of stability constants of complexes by spectrophotometric method ((Job's method) and pH –metric method(Bjerrum's).
Reactivity of metal complexes – inert and labile complexes. Explanation of lability on the basis of valence bond and crystal field theories.

UNIT- V

Reaction Mechanisms of Metal Complexes:
Reactivity of metal complexes, inert and labile complexes, Kinetics and mechanisms of substitution reactions, kinetics of substitutions reactions in octahedral complexes, acid hydrolysis, Factors affecting acid hydrolysis, Base hydrolysis, Conjugate base mechanism, Anation reactions, substitution reactions in square planar complexes, Trans effect, Mechanism of trans effect, Electron transfer reactions-– concept of complementary and non-complementary reactions with examples, inner sphere and outer sphere mechanisms, Marcus theory.

Text books:

1. Advanced Inorganic Chemistry by F.A. Cotton and R.G. Wilkinson, IV Edition, John, John Wiley and Sons, New York, 1980.
2. Inorganic Chemistry by J.E. Huheey, III edition, Harper International Edition, 1983.
3. Organometallic Chemistry-A unified approach by A. Singh and R.C. Mehrotra, Wiley Eastern Ltd.
4. Inorganic Chemistry by Shriver and Atkins, Oxford University Press (1999)
5. Theoretical Inorganic Chemistry, II Edition by M.C. Day and J. Selbin, Affiliated East-West press Pvt. Ltd., New Delhi.
6. Mechanisims of Inorganic reactions in solution by D.Benson, MCgraw Hill, London, 1968.
7. Inorganic chemistry by K.F. Purcell and J.C.Kotz, W.B. Saunders company, New York, 1977.

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Course Objectives: To make the students

CO1 Acquire the knowledge of aromaticity, aromatic nucleophilic substitution, reactive intermediates and name reactions, molecular rearrangements, spectroscopy, alkaloids, peptides, proteins and nucleic acids

CO2 Understand aromaticity, aromatic nucleophilic substitution, reactive intermediate and name reactions, molecular rearrangements, spectroscopy, alkaloids, peptides, proteins and nucleic acids

CO3 Apply the knowledge and understanding of aromaticity, aromatic nucleophilic substitution, reactive intermediate and name reactions, molecular rearrangements, spectroscopy, alkaloids peptides, proteins and nucleic acids to new situations

CO4 Develop interest in the areas of aromaticity, aromatic nucleophilic substitution, reactive intermediates and name reactions, molecular rearrangements, spectroscopy, alkaloids, peptides, proteins and nucleic acids

Learning Outcomes: At the end of the course, the learners should be able to:

LO1 Explain aromaticity, aromatic nucleophilic substitution, reactivity intermediates and name reactions, molecular rearrangements, spectroscopy, alkaloids, peptides, proteins and nucleic acids

LO2 Interpret aromaticity, aromatic nucleophilic substitution, reactive intermediates and name reactions, molecular rearrangements, spectroscopy, alkaloids, peptides, proteins and nucleic acids

LO3 Compare aromaticity, aromatic nucleophilic substitution, reactive intermediates and name reactions, molecular rearrangements, spectroscopy, alkaloids, peptides, proteins and nucleic acids

LO4 Analyse aromaticity, aromatic nucleophilic substitution, reactive intermediates and name reactions, molecular rearrangements, spectroscopy, alkaloids, peptides, proteins and nucleic acids

LO5 Solve aromaticity, aromatic nucleophilic substitution, reactive intermediates and name reactions, molecular rearrangements, spectroscopy, alkaloids, peptides, proteins and nucleic acids

LO6 Identify aromaticity, aromatic nucleophilic substitution, reactive intermediates and name reactions, molecular rearrangements, spectroscopy, alkaloids peptides, proteins and nucleic acids

LO7 Apply aromaticity, aromatic nucleophilic substitution, reactive intermediates and name reactions, molecular rearrangements, spectroscopy, alkaloids, peptides, proteins and nucleic acids

COURSE CONTENT

UNIT-I:

Aromaticity

A) **Aromaticity:** Concept of Aromaticity, Aromaticity of five membered, six membered and fused systems-non-benzenoidaromatic compounds:-cyclopropenylcation, cyclo butadienyldication, cyclopentadienyl anion — tropyliumcation and cyclo octatetraenyl dianion—matallocenes, ferrocenes, azulenes, fulvenes, annulenes, fullerenes. Homoaromaticity, Antiaromaticity and Pseudoaromaticity.

B) **Aromatic Nucleophilic Substitutions:** The SNAr, SN1, benzyne and SRN1 mechanisms. Reactivity: Effect of substrate, leaving group and attacking nucleophile. The Von-Richter, Somm1et-HauserandSmilesrearrangements.

UNIT-II:

Reactive Intermediates and Name Reactions

A) **Reactive Intermediates:** Generation, structure, stability and reactivity of reactive intermediates: carbanion, carbocation, freeradicals, carbenes and nitrenes.

B) **NameReactions:**Wittigreaction,Grignardreaction,Storkenaminereaction,Michaeladdition, MannichReaction,Diel's-AlderreactionandEne-reaction

UNIT-III:

Molecular Rearrangements

Molecular Rearrangements: Types of molecular rearrangements, migratory aptitude;

Rearrangements to electron deficient carbon: Pinacol-pinacolone, Wagner-Meerwein and Benzil-Benzilicacid,

Rearrangements toelectron deficientnitrogen: Beckmann, Hofmann, Curtius, Schmidt and Lossen rearrangements;

Rearrangements to electron deficient oxygen: Baeyer-villiger,Dakin rearrangements;

Other rearrangements: Neber rearrangement and Favorskii rearrangements

UNIT-IV:

Spectroscopy

A) **UV Spectroscopy:** Various electronic transitions, selection rules, effect of solvent on electronic transitions, the absorption laws, chromophores, auxochromes, bathochromic and hypso chromic shifts, hyperchromic and hypochromic effects, Woodward-Fieser rules for conjugated dienes and carbonyl compounds.

B) **Infrared Spectroscopy:** Basic principles: types of molecular vibrations, fingerprint region and identification of functional groups.

C) **Nuclear Magnetic Resonance Spectroscopy (^{1}H-NMR):** nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shifts, factors affecting the chemical shift, and assignment of chemical shifts.

D) **Mass Spectroscopy:** Basic principles, nitrogen rule and fragmentation pattern of carbonyl compounds and alcohols

UNIT—V:

Alkaloids, Peptides, Proteins and Nucleic acids

A) **ALKALOIDS:** Occurrence, Isolation, classification based on nitrogen heterocyclic ring and synthesis of quinine and nicotine

B) **Peptides and Proteins:** O-Amino acids, their general properties and synthesis, Synthesis of peptides by Merrifield solid phase synthesis. Primary, secondary and tertiary structures of proteins

C) **Nucleic acids**: Heterocyclic bases; Purines: Adenine and Guanine; Pyramidines: Cytosine, Uracil and Thymine; nucleosides, nucleotides Basic concepts of the structures of RNA and DNA

Textbooks:

1. Organic Chemistry Vol.I (SixthEdn.) and Vol.II (FifthEd.,) by ILfinarELBS.
2. Organic Chemistry (fifthEdn.,) by Morrison and Boyd, PHI, India.
3. Organic Chemistry (fifthedition) by FrancisA.Carey TataMcGraw Hillpublishing Company Limited, New Delhi.
4. ReactionMechanisminOrganicChemistrybyMukherjeeSirigh,NTerniit arr,Indiar
5. A guide book to mechanism in Organic Chemistry by Peter Sykes, ELBS.
6. Advanced organic chemistry by Jerry March (4thEdition)WileyEastern..
7. Stereochemistry of carbon compounds by E.Eliel, John Wiley &Sons, Inc.
8. Stereochemistry of Organic compounds by D.Nasipuri., Chemistry of Natural products by R.S. Kalsi Kalyani Publ

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Course Outcomes (COs)/Course Specific Outcomes (CSOs)

Upon completion of the course the students will be able to,

CO1 Explain the basic concepts of Crystallography

CO2 Understand the types of polymers and analyze various physical properties of polymers

CO3 Understand the concepts of electrochemistry and theories like Debye Huckel theory

CO4 Understand the basic concept and theories of electrode-electrolyte interface

CO5 Learn principles of photochemistry and various photochemical reactions

Learning Outcomes (LOs):

Upon completion of the course the student will be able

- To determine electrical magnetic properties of solids.
- To apply the basic concept of electrochemistry to different electrochemical cells
- To predict the mechanisms of photochemical reactions

COURSE CONTENT

UNIT-I:

Crystal structure of solids: Fundamental of lattices, unit cell, Bravais lattices, symmetry elements in crystals, packing efficiency, radius ratios; Miller indices. structures and types of solids. Structure determination by X-ray diffraction (Bragg's equation). Magnetic properties of solids- classification of magnetic materials, Magnetic susceptibility, Measurement of magnetic susceptibility. Electric properties-Band theory, the band structure of metals, insulators, and semiconductors. The temperature dependence of the conductivity of extrinsic semiconductors. Superconductivity and occurrence. Meisner effect. Types of superconductors. Theories of superconductivity - BCS theory.

UNIT-II

Classification of polymers - Free radical, ionic and Zeigler - Natta Polymerization - kinetics of free radical polymerization - Techniques of polymerization - Glass transition temperature - Factors influencing the glass transition temperature - Number average and Weight average, Molecular weights - molecular weights determination - End group analysis - Osmometry - Light scattering and ultra-centrifugation methods.

UNIT-III:

Electrochemistry I: Ionic mobilities and conductivities - Debye-Huckel theory of strong electrolytes, Debye-Huckelonsagar equation-limitations- mean activity coefficient - Verification of Debye-Huckel limiting law. Electrochemical cell- Galvanic and electrolytic cell. Nernst equation-Concentration cell with and without transference- effect of complexation on redox potential- ferricyanide/ ferrocyanide couple, Iron(III) phenonthroline/ Iron(II) phenonthroline couple. Fuel Cells- construction-Various types-Examples.

UNIT-IV:

Electrochemistry II: The electrode-electrolyte interface. The electrical double layer. The Helmholtz-Perrin parallel-plate model, the Gouy-Chapman diffuse-charge model and the Stern model. Electrodics: Charge transfer reactions at the electrode-electrolyte interface.Derivation of Butler-Volmer equation. High field approximation, Tafel equation, Low field equilibrium, over voltage. Theories of over voltage- Corrosion - Concentration polarization - Polarography -Half wave potential and Ilkovic equation.

UNIT-V:

Photochemistry: Electronic transitions in molecules, Franck-Condon principle. Electronically excited molecules- singlet and triplet states, spin-orbit interaction. Quantum yield and its determination. Actinometry. Derivation of fluorescence and phosphorescence quantum yields. Quenching effect- Stern Volmer equation. Photochemical equilibrium and delayed fluorescence- E-type and P-type. Photochemical primary processes, types of photochemical reactions-photodissociation, addition and isomerization reactions with examples.

Text Books:

1. Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press.
2. Physical Chemistry by G.W. Castellon, Narosha Publishing House
3. Physical chemistry by K.L. Kapoor.
4. Principles of photochemistry, RohitgeeMukhargee.

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECIALIZATION
SEMESTER-II
PRACTICAL -I: INORGANIC CHEMISTRY
(With effect from the admitted batch of 2021-2022 academic year)

Course Objectives:

CO1 To have hands-on experience/practical knowledge in Inorganic chemistry experiments
CO2 To develop skills on estimations of analyte by volumetrically
CO3 To determine analyte by Gravimetrically
CO4 To study the photochemical reactions

Learning Outcomes:

At the end of the course, the learners should be able to:

LO1 To be able to solve problems in analytical chemistry
LO2 To extend the idea of determination of analyte by volumetric titration to advanced analytical determinations of various organic and inorganic analytes
LO3 Able to design gravimetric experiments for quantitative estimation of organic and inorganic analytes

COURSE CONTENT

Quantitative analysis:

1. Volumetric methods of Analysis:

i) Determination of Ferric iron by photochemical reduction

ii). Determination of Nickel by EDTA

iii) Determination of Calcium and Magnesium in a mixture by EDTA

iv) Determination of Ferrocyanide by Ceric sulphate

v) Determination of Copper(II) in presence of iron(III)

2. Gravimetric methods of Analysis:

i) Determination of Zinc as Zinc pyrophosphate

ii). Determination of Nickel from a mixture of Copper and Nickel.

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SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECIALIZATION
SEMESTER-II
PRACTICALS -II: PHYSICAL CHEMISTRY
(With effect from the admitted batch of 2021-2022 academic year)

Course Objectives:

CO1 To have hands-on experience/practical knowledge in performing Physical chemistry experiments

CO2 To develop skills on handling instruments like Potentiometry and perform different types of acid-base and redox titrations

CO3 To determine specific rotations and percentage of to optically active substances by polarimetrically

CO4 To study the stability of complex ion and stranded free energy change and equilibrium constant by potentiometry

Learning Outcomes:

At the end of the course, the learners should be able to:

LO1 To be able to develop/practical skills to solve problems in chemistry

LO2 To extend the principle of Potentiometric titration to other kind of reactions.

LO3 To study the kinetics of reactions and determine the order of reaction

COURSE CONTENT

1. Potentiometric titration of Iron (II) using potassium dichromate
2. Potentiometric titration of strong acid with a strong base using quinhydrone electrode
3. Determination of kinetics of Ester hydrolysis
4. Determination of Equilibrium constant of Potassium Iodide-Iodine system
5. Determination of kinetics of inversion of cane sugar by polarimetry method.
6. Determination of partial molar volume of solute –H_2O system by apparent molar volume method.

TEXT BOOKS

1. A Textbook of Practical Organic Chemistry by A. I. Vogel, ELBS and Longman group.
2. Practical Organic Chemistry by Mann and Saunders, ELBS and Longman group.

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECIALIZATION
SEMESTER-II
PRACTICALS -III: ORGANIC CHEMISTRY
(With effect from the Admitted batch of 2021-2022 Academic Year)

Course Objectives:

CO1 To develop an insight into the identification of organic compounds by systematic analysis
CO2 To understand the process of identification of organic compounds by systematic analysis
CO3 To acquire skills in the identification of organic compounds by systematic analysis

Learning Outcomes:

At the end of the course, the learners should be able to:

LO1 Identify an organic compound by systematic analysis
LO2 Develop skill in identification of organic compounds by systematic analysis
LO3 Apply the skill in the identification of new organic compounds by systematic analysis

COURSE CONTENT:

Identification of the unknown organic compounds

Systematic identification of organic compounds – preliminary tests, detection of extra elements, solubility, common functional group tests (determination of functional group/s in a single compound, if present), preparation of two rational derivatives

The given organic compound must be identified by comparing the melting point /Boiling point of the compound and melting points of its derivatives with the literature

List of suggested compounds

Glucose, fructose, benzaldehyde, p-anisaldehyde, p-chloro benzaldehyde, acetophenone, phenol, cresols, naphthols, esters, p-chloro benzoic acid, aniline, p-tolune, p-anisidine, p-chloroaniline, diphenyl amine, N,N-dimethylaniline, benzamide, naphthalene and anthracene.

MODEL QUESTION PAPER
ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECIALIZATION
SEMESTER - II
PAPER I: GENERAL CHEMISTRY-II
(With effect from the Admitted batch of 2021-2022 Academic Year)

Time: 3 Hours **Max. marks: 80 (5X16 =80 marks)**

Answer ALL questions

(1) (a) i) Derive Schrodinger wave equation?
ii) Explain the postulates of Quantum mechanics
(or)
(b) i) Write notes on Hermitian operator and its properties
ii) Explain normalization and orthogonalization

(2) (a) i) Solve the Schrodinger wave equation for a particle in a one-dimensional box
ii) Write the factors influencing color
(or)
(b) i) Derive the Schrodinger wave equation for a simple harmonic oscillator
ii) Describe the concept of tunnelling

(3) (a) i) Explain the solution of R(r), $\theta(\theta)$ and $\Phi(\phi)$ equations of hydrogen atom
ii) Explain probability density in orbitals
(or)
(b) i) Explain the time independent perturbation theory to evaluate the ground state energy of helium atom
ii) Application of above to ground state energy of hydrogen and helium atom

(4) (a) i) What is variation principle. Write its application to calculation of ground state energy of harmonic oscillator
ii) Compare Perturbation and variation theorems
(or)
(b) i) Explain Hartee-Fock self-consistent field method for multi electron atoms
ii) Write a note on Density functional theory (DFT)

(5) (a) i) Explain quantum mechanical approach of molecular orbital theory
ii) Calculate the ionic and covalent bond contributions in hydrogen molecule
(or)
(b) i) Discuss the valence bond approach of H_2 molecule.
ii) Write the electronic transitions in the hydrogen molecule.

MODEL QUESTION
ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECIALIZATION
SEMESTER-II
PAPER- II: INORGANIC CHEMISTRY-II
(With effect from the Admitted batch of 2021-2022 Academic Year)

Time: 3 Hours **Max marks: 80 (5X16 =80M)**

Answer ALL questions

(1) a) (i) Discuss the structure and magnetic property of $Cu_2(RCOO)_4(H_2O)_2$
(ii) Write a note on Chevrel phases
(or)
b) (i) Discuss the preparation of, structures of and bonding in $Re_2Cl_8^{2-}$.
(ii) Describe the structures of hexanuclear metal clusters

(2) a) (i) Explain the synthesis, structure and reactions of metal carbonyls.
(ii) Explain Isolobal relationship with suitable examples.
(or)
b) (i) Describe the preparation of, structure of and bonding in ferrocene.
(ii) What is 18 electron rules? Illustrate with suitable examples

(3) a) (i) Explain the factors affecting the stability of coordination compounds
(ii) Distinguish between stepwise and overall stability constants
(or)
b) (i) Describe the Irwing-William's series, Pearson's theory of hard and soft acids and bases (HSAB)
(ii) What is chelate effect and discuss its thermodynamic origin

(4) a) (i) Discuss a spectrophotometric method for the determination of binary formation constant of a metal complex
(ii) What are inert and labile complexes?
(or)
b) (i) Describe the pH – metric method for the determination of stability constants
(ii) Explain inert and labile complexes by using crystal field stabilization energies?

(5) a) (i) What is acid hydrolysis reactions? Discuss factors affecting acid hydrolysis reactions
(ii) What is trans effect? Distinguish between the trans effect and trans influence
(or)
b) (i) Give an account of base hydrolysis of Cobalt (III) complexes
(ii) Discuss the various factors affecting the rates of substitution reaction of octahedral complexes

MODEL QUESTION
ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECIALIZATION
SEMESTER-II
PAPER- III: ORGANIC CHEMISTRY-II
(With effect from the Admitted batch of 2021-2022 Academic Year)

Time: 3 Hours **Maximum marks: 80 (5X16 =80 marks)**

Answer ALL questions

(1) a) (i) Explain Aromaticity and Anti aromaticity give examples.
(ii) Write a note on Von- Ritcher rearrangement
(or)
b) (i) Describe Aromatic Nucleophilic Substitution reactions give examples.
(ii) Write a note on Non-benzenoid aromatic compounds and Annulenes.

(2) a) (i) Write any two preparations and reactivity of carbocation.
(ii) Write a note on Stork enamine reaction.
(or)
b) (i) Explain carbanion and nitrene
(ii) Briefly explain Mannich Reaction with applications.

(3) a) (i) Explain Pinacol-pinacolone rearrangement give examples.
(ii) Describe mechanism and applications of Beckmann rearrangement.
(or)
b) (i) Discuss about Baeyer-villager rearrangement.
(ii) Write a note on Favorskii rearrangement.

(4) a) (i) Write the Woodward-Fieser rules for conjugated dienes.
(ii) Explain types of molecular vibrations in Infrared Spectroscopy.
(or)
b) (i) Describe factors affecting the chemical shift.
(ii) Give the fragmentation pattern of alcohols.

(5) a) (i) Write the synthesis of nicotine
(ii) Explain Merrifield solid phase synthesis.
(or)
b) (i) Write about Primary, secondary and tertiary structures of proteins.
(ii) How do you differentiate RNA and DNA

MODEL QUESTION
ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECIALIZATION
SEMESTER-II
PAPER- IV: PHYSICAL CHEMISTRY-II
(With effect from the Admitted batch of 2021-2022 Academic Year)

Time: 3 Hours **Max. Marks: 80 (5X16 =80M)**

Answer ALL questions

(1) a) (i) Derive Bragg's equation
(ii) Explain the theories of superconductivity
(or)
b) (i) Describe the different methods of measurement of magnetic susceptibility
(ii) Write a brief note on semiconductors

(2) a) (i) Give the classification of polymers with examples
(ii) What are the factors influencing glass transition temperature
(or)
b) (i) How is molecular weight of polymers determined by osmometry and light scattering methods
(ii) Write a brief note on kinetics of free radical polymerization

(3) a) (i) Explain Debye-Huckel theory of strong electrolytes
(ii) Discuss the effect of complexation on redox potential with examples?
(or)
b) (i) Derive an expression for EMF of concentration cell without transference
(ii) Discuss the important features of Debye-Huckel limiting law

(4) a) (i) Derive Bulter-Volmer equation
(ii) Explain the Stern model for double layer
(or)
b) (i) Explain in detail about polarography
(ii) Discuss important features of Gouy-Chapman diffuse charge model and Helmholtz parallel plate model
(or)
(5) a) (i) Derive Stern-Volmer equation
(ii) State and explain Franck-Condon principle

b) (i) Define quantum yield and explain its experimental method determination
(ii) Discuss the mechanism of photo addition and photo isomerization with examples

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZATION
THIRD SEMESTER
(Effective from the admitted batch of 2021-2022)

PO1 To master knowledge in the principal areas of Physical chemistry
PO2 To be competent in solving industrial scientific problems through experimental, computational and/or data analysis models
PO3 To indulge in deeper learning of the principles of thermodynamics, quantum chemistry, Kinetics and molecular symmetry and group theory.
PO4 To learn modern spectroscopic tools and their applications to different disciplines of chemistry
PO5 To design and conduct experiments as well as to analyse and interpret the data
PO6 To work effectively both as an individual and as a collaborative team member
PO7 To appreciate the importance of goal-setting and to recognize the need for life-long reflective learning
PO8 To learn, design and demonstrate sustainable industrial reactions within realistic constraints such as economic, environmental considerations.

PSO1 Students will learn the advanced thermodynamic concepts and its applications.

PSO2 Students will grasp the solutions of quantum mechanical problems

PSO3 Students will learn the applications spectroscopy
PSO4 Competency to clear competitive examinations like CSIR-NET, GATE and BARC etc…
PSO5 Develops analytical skills and problem solving skills requiring application of chemical principles
PSO6 Have sound knowledge about the fundamentals and applications of chemical and scientific theories

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZATION
THIRD SEMESTER
PAPER–I POLYMER CHEMISTRY AND PHOTOCHEMISTRY
(With effect from the Admitted batch of 2021-2022 Academic Year)

Course Outcomes (COs)-Course Specific Outcomes (CSOs)

Upon completion of the course the students will be able to,

CO1: Explain the different mechanisms of polymerization process

CO2: Determine Number, weight and viscosity average molecular weights with various techniques

CO3: Make use of the concepts polymer blend and Nano composites and its applications

CO4: Understand the basic concepts of photochemistry and photochemical stages

CO5: Solve various problems on photochemical transformations.

LearningOutcomes (LOs):

Upon completion of the course the student will be able to

- Predict mechanism of polymerization reactions.
- Determine mechanical properties of polymers.
- Useprinciples of photochemistry to different organic reactions.
- Predict the structure of organic compounds.
- Understand the importance of polymer blend and Nano composites

CO-PO MAPPING

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	✔	✔			✔	✔	✔	✔
CO2	✔	✔			✔	✔	✔	✔
CO3	✔	✔			✔	✔	✔	✔
CO4	✔	✔			✔	✔	✔	✔
CO5	✔	✔			✔	✔	✔	✔

COURSE CONTENT

UNIT-I

Polymer Synthesis: Step, chain and miscellaneous polymerizations- Kinetics of polymerization. Anionic, Cationic, ATRP, ROMP, RAFT, Free radical polymerization- Polymerization of cyclic organic compounds - Reactions of synthetic polymers - Biological polymers - Inorganic elements in polymers- State of Polymerization: Emulsion, Dispersion, Solution, Solid-state etc.

UNIT-II

Molecular Weights and Sizes: Solubility parameters, Flory-Huggins Theory for polymer solution, Flory-Huggins parameter, Polymer shape and size, measurement techniques-viscosity, colligative properties, chromatography, light scattering (Zimmplot)-Physical State and Morphology: Crystalline

and Amorphous state- Thermal transitions- Glass Rubber transition - Mechanical properties− stress-strain behavior - Elastomer, Fibers and Plastics

UNIT-III

Polymer Blend and Nano composites: Preparation, Types of blends, types of nano fillers, Thermo dynamical considerations, Property enhancements, Uses. Application of Synthetic Polymers: Materials and Biological importance and uses. Nano materials, Conducting polymers, Polymers for Energy applications.

UNIT-IV

Photochemistry: Absorption Excitation – photochemical laws – quantum yield of electronically excited states – measurements of life times – Flash photolysis – Stopped flow Technique - energy dissipation by radiative and non-radiative processes, absorption spectra – Franck-Condon principle. Photochemical stages – Primary processes and secondary processes – Rate constants and life times of reactive excited states.

UNIT-V

Properties of excited states: structure, dipole moment acid base strengths – reactivity, kinetics of bimolecular processes – quenching, Stern-Volmer equation. Photo reduction and photo oxidation.Cyclo addition reactions, Wood-ward-Hofmann's rules.

Suggested Books:

1. W. R. Moore-An introducer to polymer chemistry.
2. Introducer to polymer Chemistry-R. B. Seymour.
3. Photochemistry – Cox and Kemp.
4. K. K. Rohatgi-Mukherjee. Fundamentals of Photochemistry. Reprint 2002. New Age International Publisher, 1978.-
5. P. Bahadur and N. V. Sastry, Principles of Polymer Science, second edition, Narosa Publishing House, 2005.
6. C. E. Carraher, Jr., Carraher's Polymer Chemistry, 8th edition, CRC Press, New York, 2010.
7. V. R. Gowarikar, H. V. Viswanathan and J. Sreedhar, Polymer Science. New Age International Pvt. Ltd., New Delhi, 1990.
8. F. W. Billmeyer Jr., Text Book of Polymer Science, 3rd edition, John Wiley and Sons, 1984.
9. V. K. Ahluwalia& A. Mishra. Polymer Science, A text book, Ane Books Pvt. Ltd, 2008.

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZATION
THIRD SEMESTER
PAPER–II QUANTUM CHEMISTRY-II AND CHEMICALAPPLICATIONS OF SYMMETRY AND GROUP THEORY

(With effect from the Admitted batch of 2021-2022 Academic Year)

Course Outcomes (COs)-Course Specific Outcomes (CSOs)
Upon completion of the course the students will be able to,
CO1: Solve various problems of wave mechanics of simple systems.
CO2: Understand the concepts of shapes of atomic orbitals and commutative relations.
CO3: Make use of the concepts variation methods and its applications.
CO4: Explain the applications of symmetry and group theory to chemical bonding.
CO5: Explain the applications of symmetry and group theory to spectroscopy.

Learning Outcomes (LOs):
Upon completion of the course the student will be able to
- Solve the Schrodinger wave equation for different problems.
- Use approximation methods in quantum chemistry.
- Apply the concepts of symmetry and group theory to various chemical problems.

CO-PO MAPPING

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	✔	✔	✔		✔	✔	✔	✔
CO2	✔	✔	✔		✔	✔	✔	✔
CO3	✔	✔	✔		✔	✔	✔	✔
CO4	✔	✔	✔		✔	✔	✔	✔
CO5	✔	✔	✔		✔	✔	✔	✔

COURSE CONTENT

UNIT-I
Wave mechanics of simple systems-System with discontinuity in the potential field- Quantum mechanical tunneling effect-potential barrier with finite thickness.
Wave mechanics of system with variable potential energy-Harmonic Oscillator-Hermite polynomials recursion formula-Energy levels of three dimensional harmonic oscillator-degeneracy of the energy levels.

UNIT-II
Hydrogen like atoms-Solution of the wave equation-solution of R(r), Φ (φ) and θ (θ) equations- Shapes of atomic orbitals-Space quantization of electronic orbitals.
Angular momentum-Commutation relations with Hamiltonian-Spin-Orbit interaction-Vector model of the atom.

UNIT-III

Approximation method-Variation method and its application-Linear and non-linear variation functions-Ground state of hydrogen atom-Ground state of helium atom- ground state energy of one-dimensional harmonic oscillator-Calculation of Eigen functions of Hamiltonian operators.

UNIT-IV

Group Theory- Representations-reducible and irreducible representations-Orhogonality theorem and its consequences-Constructions of Character tables for C_{2V} and C_{3V} point groups- wave functions as bases for irreducible representations- Direct product.
Applications to Chemical Bonding-Hybridization scheme for AB_n type of molecules- AB_3, AB_4, AB_5 and AB_6 under point groups D_{3h}, D_{4h}, T_d, C_{4v} and O_h.
Ligand field theory: splitting of d-orbitals under D_{4h}, T_d, C_{4v} and O_h environments.

Construction of molecular orbital correlation diagram (1) for σ bonds in octahedral environment and (2) for H_2O molecule.

UNIT-V

Applications to Molecular Vibrations:

Symmetry selection rules for IR and Raman activity – transition moment integral- application of direct product - Determination of symmetries of total degrees of freedom: calculation of Character per un-shifted atom for different symmetry operations and evaluation of Γ_{3N}.

Determination of symmetries of IR and Raman active vibrational modes for different molecules – SO_2, NO_3^-, ClO_4^-, $POCl_3$, $POCl_4$ and SF_6.

Accidental degeneracy and Fermi Resonance.

Recommended Text Books:

1. Chemical Applications of Group Theory, F. A. Cotton Wiley Eastern Limited New Delhi.
2. Group Theory and its Applications to Chemistry, K. V. Raman, Tata McGraw – Hill Publishing Company Ltd., New Delhi.
3. K. Veera Reddy, Symmetry and Spectroscopy of molecules, 2nd ed, new age International publishers.
4. Bhattacharya, Group theory and its chemical applications, 1999, Himalaya, Pub. House.
5. Symmetry and Group theory-Vincent
6. I.N. Levine, Quantum Chemistry, 5 th edition (2000), Pearson Educ. Inc., New Delhi.
7. D.A. McQuarrie and J.D. Simon, Physical Chemistry: A Molecular Approach, (1998) Viva Books, New Delhi.
8. A.K. Chandra, Introductory Quantum Chemistry, 4th edition (1994), Tata McGraw Hill, New Delhi.
9. D. A. McQuarrie, Quantum Chemistry, Viva Books Private Limited, New Delhi, first Indian ed., 2003.
10. R. K. Prasad, Quantum Chemistry, 3rd Ed., New Age International Publishers, 2006.

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZATION
THIRD SEMESTER
Paper–III STATISTICAL THERMODYNAMICS AND SOLUTION EQULIBRIA OF METAL COMPLEXES
(With effect from the Admitted batch of 2021-2022 Academic Year)

Course Outcomes (COs)-Course Specific Outcomes (CSOs)
Upon completion of the course the students will be able to,
CO1: Develop the tools of statistical mechanics.
CO2: Understand basic concepts of partition function and calculation of entropy.
CO3: Make use of the concepts of stability constants of proton –ligand complexes.
CO4: Understand the different titration techniques of meta-ligand complexes.
CO5: Understand the basic components and principles of expert systems.

Learning Outcomes (LOs):
Upon completion of the course the student will be able to
- Use basic principles of statistical thermodynamics in predicting bulk thermodynamic functions
- Acquire knowledge in MINIQUAD program.
- Provide stability constants of Metal-Ligand complexes
- Use Trojan software

CO-PO MAPPING

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	✔	✔			✔	✔	✔	✔
CO2	✔	✔			✔	✔	✔	✔
CO3	✔	✔			✔	✔	✔	✔
CO4	✔	✔			✔	✔	✔	✔
CO5	✔	✔			✔	✔	✔	✔

COURSE CONTENT

UNIT –I

Statistical mechanics: Ensembles (Canonical and micro canonical) – Basic definition distribution and microstates, thermodynamic probability. The classical distribution law. The Maxwell – Boltzmann distribution law, method of Lagrangian multipliers, indistinguishable particles, quantum statistics – Bose – Einstein and Fermi Dirac Statistics, Conditions for the applicability of Maxwell – Boltzmann statistics, Bose-Einstein statistics and radiation, extreme gas degeneration, degenerate electron gas.

UNIT –II

Statistical thermodynamics:Partition functions-Equilibrium constants in terms of partition coefficient Thermodynamics functions from partition functions for multiple degree of freedom, Einstein and Debye models of heat capacities of solids, statistical evaluation of entropy, comparison of statistical values with third law entropies (thermal entropies)

UNIT –III

Gran analysis of acid base titrations- Determination of Carbonate content and correction factors for pH meter dial readings;Secondary formation function nbarh;Calculation of stability constants of proton

ligand complexes-successive approximation method-half nbarh method; Simulation of pH metric titration data for proton-ligand systems. Prediction of proton-ligand formation constants using Molecular mechanics/ Quantum Chemical methods; Effect of solvent on stability –Abraham multi-layer model – LD model.

UNIT - IV

Calvin Wilson Titration Techniques for metal ligand complexes –Determination of stability constants using formation function, hydroxylated complexes stability constant by Martell method – Laden procedure. Solution of a non – linear function of two variables – Algorithm of MINIQUAD programme – criteria of best fit model input/output.

UNIT – V

Prediction of metal ligand stability constants- Irving and William order. Components of expert systems – knowledge base, inference engine and user interface.Neural networks – Processing element, Transfer function, Training algorithm – BFGS, MAFQUARDT and back propagation.Multilayer perception and radial basis function NN's.Features of Trajan software – Input Output – Intelligent problem solver.

Suggested Books:

1. M. T. Beck, Complex Equilibria, 1991
2. Alcock, solution Equilibria, 1992
3. Richard E. Dickerson, Molecular Thermodynamics
4. S. Glasstone, Thermodynamics for Chemists
5. C. Andrews, Equilibrium Statistical Mechanics.
6. John M. Seddon& Julian D. Gale, Thermodynamics and statistical mechanics.
7. Silbey R J &Alberty R A, Physical Chemistry, 3rd edition, John Wiley and sons, Inc.2002.
8. Laidler K.J. and Meiser J. H., Physical Chemistry, 2nd edition, CBS publishers & distributors,1999.
9. B.K. Agarwal and M. Eisner, Statistical Mechanics, (1988) Wiley Eastern, New Delhi.
10. D. A. McQuarrie, Statistical mechanics, (1976) Harper and Row Publishers, New York.

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZATION
THIRD SEMESTER
PAPER–IV INSTRUMENTATION
(With effect from the Admitted batch of 2021-2022 Academic Year)

Course Outcomes (COs)-Course Specific Outcomes (CSOs)

Upon completion of the course the students will be able to,

CO1: Explain the instrumentation and applications different chromatographic techniques like Gas-liquid, HPLC, GC etc.,

CO2: The student will acquire qualitative and quantitative knowledge of the fundamental concepts of various spectrochemical methods,

CO3: Understand basic concepts and detailed applications of spectroscopic methods

CO4: Understand the different electrochemical methods

CO5: Understand the principles of different thermal methods like gravimetry, TGA, and DTA etc.,

Learning Outcomes (LOs):

Upon completion of the course the student will be able to

- Extend the knowledge of separation techniques to various types of analytes.
- Apply the spectrochemical and spectroscopic techniques like UV-VIS, AAS and AES to various compounds.
- Use electrochemical methods like polarography, voltammetry and cyclic voltammetry to study the organic and inorganic compounds.
- Use electro thermal methods like thermo gravimetric analysis and differential thermal analysis to analyze the organic, inorganic compounds and drugs.

CO-PO MAPPING

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	✔	✔			✔	✔	✔	✔
CO2	✔	✔			✔	✔	✔	✔
CO3	✔	✔		✔	✔	✔	✔	✔
CO4	✔	✔			✔	✔	✔	✔
CO5	✔	✔			✔	✔	✔	✔

COURSE CONTENT

UNIT-I

Separation techniques-different types, applications, solid phase extraction.Ion exchange-principle, separation of transition metal ions and other applications - ion chromatography – Gas liquid chromatography (GLC) - principle - instrumentation- application, ion chromatography- HPLC – principle – applications-Reverse phase HPLC - applications.

UNIT-II

Spectrochemicalmethods:Spectrophotometry, Beer-Lambert's law and deviations, errors in spectrophotometry. Instrumentation and applications, photometric titrations.Fundamental principles of fluorescence spectroscopy and basic instrumentation of a spectrofluorimeter.Atomic absorption spectroscopy- Principle, Instrumentation and applications-Atomic emission spectrometry with ICP source-principle, instrumentation and applications.

UNIT-III

Spectroscopic methods:Mass spectrometry, Ion sources-thermal ionization, electron impact ionization. Magnetic analysers, quadrupoleanalysers, time of flight analysers. Elementary principles of laser mass spectrometry. Introduction to hyphenated instruments like GC-MS andHPLC-MS.Instrumentation of IR, Raman and Microwave spectroscopy and applications.

UNIT-IV

Electrochemical methods:Polarography-Introduction-types of currents-qualitative and quantitative aspects of polarography-analytical application to organic and inorganic compounds-amperometric titrations. Half-wave potential, Ilkovic equation,Dropping mercury electrode (DME)-Principle and applications of cyclic voltammetry, anode stripping voltammetry and Coulometric analysis.

UNIT-V

Thermal methods of Analysis- Thermo gravimetry-theory, instrumentation, applications with special reference to$CuSO_4.5H_2O$, $CaC_2O_4.2H_2O$, $CaCO_3$, $(COOH)_2$ $2H_2O$-Differential thermal analysis-principle, instrumentation, difference between TGA andDTA. Factors affecting TGA and DTA curves-applications-Differential scanning calorimetry- principle, instrumentation, applications to inorganic and organic compounds and drugs.

Suggested Books:

1. Instrumental Methods of Analysis, H. H. Willard, L. L. Merritt, Jr., J. A. Dean, F. A. Settle, Jr. CBS Publishers and Distributors, New Delhi 1986.
2. Quantitative Analysis-R.A Day and A. L. Underwood.
3. Quantitative Inorganic Analysis-A. I. Vogel.
4. Principles of Instrumental analysis, D. A. Skoog, F. J. Hollers, S. R. Crouon.
5. Instrumental methods of chemical analysis, Gurudeep R. Chatwal, Sham K. Anand Himalaya Publishing House.
6. Skoog D A, West D M , Fundamentals of Analytical Chemistry, Thomson Asia Pvt ltd., 8 th Ed, (2004)

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZATION
THIRD SEMESTER
PRACTICAL-I: KINETICS
(With effect from the Admitted batch of 2021-2022 Academic Year)

Course Objectives (COs):

Upon completion of the course the students will be able to,

CO1: Maintain laboratory ethics, safety and cleanliness.

CO2: Preparation and standardization of solutions.

CO3: Have hands-on experience/practicalknowledge in performing advanced physical chemistry experiments

CO4: Develop skills on handling instruments like conductometer, potentiometer and pH meter and perform different types of titrations

CO5: Develop skills in procedures and instrumental methods applied in analytical and practical tasks of physical chemistry

CO6: Develop some understanding of the professional and safety responsibilities residing in working with chemical systems.

Learning Outcomes (LOs):

At the end of the course, the learners should be able to:

LO1: Develop practical skills to solve problems in chemistry.

LO2: Extendthe applications of conductometric, potentiometric and pH metric titrations to other kind of reactions.

LO3: Learn the order and molecularity of different chemical reactions

LO4: Extend the experimental methods of rate law determination

LO5: Apply the effect of ionic strength to different chemical reactions

COURSE CONTENT

1. Saponification of ester.
2. Saponification of ester by Conductometry.
3. Effect of ionic strength on persulphate-iodide reaction.
4. Ester hydrolysis.
5. Iodine clock Reaction.
6. Determination of Partial molar volumes of methanol in dilute aqueous solutions

TEXT BOOKS:

1. A Textbook of Practical Physical Chemistry experiment by Gurtu-Grutu
2. Experiment in Physical Chemistry by Carl w.Garland, Joseph w.Nibler, McGraw-Hill

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZATION
THIRD SEMESTER
PRACTICAL-II: INSTRUMENTATION
(With effect from the Admitted batch of 2021-2022 Academic Year)

Course Objectives (COs):

Upon completion of the course the students will be able to,

CO1: Maintain laboratory ethics, safety and cleanliness.

CO2: Preparation and standardization of solutions.

CO3: Have hands-on experience/practicalknowledge in performing advanced physical chemistry experiments

CO4: Develop skills on handling instruments like conductometer, potentiometer and pH meter and perform different types of titrations

CO5: Develop skills in procedures and instrumental methods applied in analytical and practical tasks of physical chemistry

CO6: Develop some understanding of the professional and safety responsibilities residing in working with chemical systems.

Learning Outcomes (LOs):

At the end of the course, the learners should be able to:

LO1: Develop practical skills to solve problems in chemistry.

LO2: Extendthe applications of conductometric, potentiometric and pH metric titrations to other kind of reactions.

LO3: Learn the order and molecularity of different chemical reactions

LO4: Extend the experimental methods of rate law determination

LO5: Apply the effect of ionic strength to different chemical reactions

COURSE CONTENT

1. Conductometric titrations of $HCl+CH_3COOH+CuSO_4$vsNaOH.
2. Potentiometric titration of Mn(VII),V(V) with Fe(II).
3. Potentiometric titrations of Ce(IV),V(V) with Fe(II).
4. Estimation of HCl by NaOH using pH meter.
5. Dissociation constant of H_3PO_4 by using pH meter.
6. Verification of Debye- Huckel Onsager equation.

TEXT BOOKS:

1. A Textbook of Practical Physical Chemistry experiment by Gurtu-Grutu

2. Experiment in Physical Chemistry by Carl w.Garland, Joseph w.Nibler, McGraw-Hill

MODEL QUESTION PAPER
ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZATION
THIRD SEMESTER
PAPER – I: POLYMER CHEMISTRY AND PHOTO CHEMISTRY
(With effect from the Admitted batch of 2021-2022 Academic Year)

Time:3hours **Max. Marks: 80M**

ANSWER ALL QUESTIONS (5 ×16 = 80)

1. (a) Discuss the mechanism involved in anionic, cationic and free radical polymerization withexamples.
(b) Discuss the kinetics of free radical Polymerization.

(or)

2. (a) Write a note on Biological polymerization.
(b) Explain polymerization of cyclic organic compounds.

3. (a) Explain Flory-Huggins theory of polymer solutions.
(b) Explain about Glass rubber transition of polymers.

(or)

4. (a) How is molecular weight determined by colligative property method and light scattering method.
(b) Define number average and weight average molecular weight of polymers and write the relation.

5. (a) Discuss biological importance and uses of synthetic polymers with applications.
(b) Discuss the applications of conducting polymers.

(or)

6. (a) Explain different types of blends and nanofillers.
(b)Write a detail note on polymers with respect to energy applications.

7. (a) Explain photochemical laws and discuss quantum yield of electronically excited states.
(b) How the rate constants and life times of reactive exited states are determined.

(or)

8. (a) Write a note on Frank-Condon principle.
(b)What is the principle involved in Flash photolysis.

9. (a) Explain Cycloaddition reactions with examples.
(b) Discuss Wood-ward-Hofmann's rules with examples.

(or)

10. (a) Derive Stern-Volmer equation along with an expression for K_{SV}.
(b) Explain Photo reduction and oxidation with examples.

MODEL QUESTION PAPER
ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZATION
THIRD SEMESTER
PAPER – II: QUANTUM CHEMISSTRY –II AND CHEMICAL APPLICATIONS OF SYMMETRY AND GROUP THEORY
(With effect from the Admitted batch of 2021-2022 Academic Year)

Time: 3 hours **Max. Marks: 80M**

ANSWER ALL QUESTIONS (5×16=80)

1. (a) Give detailed account of quantum mechanical tunneling effect?
   What are the different shapes of barriers for tunneling?
   (b) Explain Hermite polynomial recursion formula.

(Or)

2. (a) Derive the solution of simple harmonic oscillator in quantum mechanics and explain its application.
   (b) Discuss the degeneracy of energy levels in simple harmonic oscillator.
3. (a) Derive the solution of Schrödinger wave equation for hydrogen atom. Explain how it is solved?
   (b)Give a detailed note on space quantization of electronic orbitals.

(Or)

4. (a) Give a detailed account of vector model of the atom.
   (b) Write a note on spin-orbit interaction in quantum mechanics.

5. (a) State and explain Variation method and explain the application of variation method to ground state energy of Helium atom
   (b) Explain Non-linear variation method with examples

(Or)

6. (a) How is Eigen function of Hamiltonian operators for harmonic oscillator using variation method
   (b) Derive the solution of ground state energy of hydrogen atom using variation method

7. (a) Construct the molecular orbital correlation diagram for sigma bonds in octahedral environment
   (b) State and explain Orthogonality theorem

(Or)

8. (a) Discuss splitting of d-Orbitals under D_{4h} environment using group theory.
   (b) Explain hybridization. Discuss the hybridization scheme for BF_3 molecule.

9. (a) Determine the symmetries of IR and Raman active vibrational modes for SO_2 and NO^-_3molecules
   (b) Write a note on accidental degeneracy

(Or)

10. (a)Determine the symmetries of IR and Raman active vibrational modes for SF6 molecules
    (b) Write a brief note on direct product and its applications.

MODEL QUESTION PAPER
ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZATION
THIRD SEMESTER
PAPER – III: STATISTICAL THERMODYNAMICS AND SOLUTION EQUILIBRIA OF PROTON – LIGAND COMPLEXES
(With effect from the Admitted batch of 2021-2022 Academic Year)

Time: 3 hours **Max. Marks: 80M**

ANSWER ALL QUESTIONS (5×16=80)

1. (a) Explain the method of Lagrangian multipliers. Derive Boltzmann distribution law.

   (b) Discuss different types of ensembles

(Or)

2. (a) Give an account of Fermi Dirac statistics and Bose-Einsteinstatistics with suitable examples.

   (b) Write a note on degenerate electron gas concept in statistical thermodynamics.

3. (a) Derive an expression for translational and rotational partition functions.

   (b) Discuss the comparison between statistical entropies and thermal entropies

(Or)

4. (a) Discuss the theories of heat capacities of solids based on statistical thermodynamics.

   (b) Derive an expression for vibration partition function.

5. (a) Explain half n barh method and successive approximation methods for calculation of stability constants of Proton-Ligand complexes

   (b) How to simulate pH metric titration data for proton-Ligand systems.

(Or)

6. (a) Describe the Abraham multilayer model and LD model to explain the effect of solvent on stability constants.

   (b) Explain how the proton-Ligand formation constants are predicted using quantum mechanical methods

7. (a) Describe the Calvin-Wilson titration technique for the experimental determination of formation function.

   (b)Explain briefly about Martell method

(Or)

8. (a) Write the algorithm of MINIQUAD programme.

   (b)Explain briefly about Laden method

9. (a) Discuss the salient features of Trajan software

   (b) How do you predict the metal ligand stability constants by Irving and William Order?

(Or)

10. (a) Explain briefly about the components of expert system

    (b) Write a detailed note on multilayer perception and radial basis function neural networks

MODEL QUESTION PAPER
ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZATION
THIRD SEMESTER
PAPER-IV: INSTRUMENTATION
(With effect from the Admitted batch of 2021-2022 Academic Year)

Time:3hours **Max. Marks: 80M**

ANSWER ALL QUESTIONS (5 ×16 = 80)

1. (a) Describe principle and instrumentation of HPLC using diagram.

. (b) Explain the principle of solid phase extraction along with applications.

(or)

2. (a) Write a note on ion-exchange chromatographyand its use in separation of lanthanides and actinides.
   (b) Describe the instrumentation of Gas liquid chromatography.

3. (a) Discuss fundamental principle of fluorescence spectroscopy and basic instrumentation of a Spectrofluorimeter.

   (b) What are the different type atomization techniques?

(or)

4. (a) Explain about Beer – Lamberts law and its limitations.
   (b) Write a note on Atomic emission spectrometry with special reference to ICP.

5. (a) Explain the instrumentation of Microwavespectroscopy.

   (b) Describe function quadrupole and time of flight analyzers.

(or)

6. (a) Explain the applications of Ramanspectroscopy.
   (b) What is principle of GC-MS hyphenate techniques.

7. (a) Describe principles and applications of Cyclic voltammetry.
   (b) What are the advantages and disadvantages of DME?

(or)

8. (a) Describe the principle of Amperometric titrations.
   (b) What is the principle of Coulometry and mention its uses.

9. (a) Discuss principle and instrumentation of Differential thermal analysis.
   (b) Discuss applications of TGA.

(or)

10. (a) Explain principle and instrumentation of TGA.
    (b) What the factors affecting TGA curve.

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZATION
FOURTH SEMESTER
(With effect from the Admitted batch of 2021-2022 Academic Year)

PROGRAMME OUTCOMES

PO1 To master knowledge in the principle areas of Physical chemistry
PO2 To demonstrate competence in solving scientific problems through experimental, computational models.
PO3 To learn the principles of non-equilibrium thermodynamics, quantum chemistry, Kinetics, FORTRAN programming.
PO4 To learn modern spectroscopic tools and their applications to different disciplines of chemistry.
PO5 To conduct experiments and analyse and interpret the data.
PO6 To create an awareness of the impact of chemistry on the environment.
PO7 To recognize the need for life-long reflective learning.
PO8 To learn, design and demonstrate sustainable industrial reactions within realistic constraints such as economic and environmental considerations.

PROGRAMME SPECIFIC OUTCOMES

PSO1 Students will learn the thermodynamic concepts and its applications.
PSO2 Students will grasp the solutions of quantum mechanical problems and its applications.
PSO3 Students will learn to know the applications of symmetry and group theory problems.
PSO4 Competency to clear competitive examinations like CSIR-NET, GATE, ONGC and BARC etc…
PSO5 Develops analytical skills and problem solving skills requiring application of chemical principles.
PSO6 Have sound knowledge about the fundamentals and applications of chemical and scientific theories.

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZATION
FOURTH SEMESTER
PAPER-I ADVANCED CHEMICAL KINETICS AND PHYSICAL-ORGANIC CHEMISTRY
(With effect from the Admitted batch of 2021-2022 Academic Year)

Course Outcomes (COs)-Course Specific Outcomes (CSOs):
Upon completion of the course the students will be able to,
CO1: Explain the kinetics of different theories, complex reactions and fast reactions
CO2: Understand the electron transfer and catalysis reactions.
CO3: Make use of the concepts of acidity functions and substitutions reactions in octahedral complexes.
CO4: Understand the basic concepts of linear free energy relationships and Huckel theory
CO5: Solve various thermodynamic and kinetic principles in principles.

LearningOutcomes (LOs):
Upon completion of the course the student will be able to
- Determine reaction rates based on Transition state theory
- Apply Marcus theory to various reaction rates.
- Predict reaction mechanism usingphysical-organic chemistry concepts.

CO-PO MAPPING

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	✔	✔			✔	✔	✔	✔
CO2	✔	✔			✔	✔	✔	✔
CO3	✔	✔			✔	✔	✔	✔
CO4	✔	✔			✔	✔	✔	✔
CO5	✔	✔			✔	✔	✔	✔

COURSE CONTENT

UNIT – I

Theories of reaction rates-Potential energy surfaces-reaction coordinate - Theories of Unimolecular gas phase reactions- Lindeman hypothesis-Hinshelwood treatment- RRKM theory- Chain reactions H_2-Cl_2, H_2-Br_2, H_2-O_2reaction-explosion limits- Complex reactions-Consecutive- Parallel and opposing reactions-Equilibrium and steady state technique- Flow and relaxation technique for fast reactions-NMR methods determining exchange rates.

UNIT-II

Marcus Theory of electron transfer adiabatic and non-adiabatic electron transfer – outer and inner sphere mechanism – effect of solvent on rates – effect of dielectric constants on ion – ion, ion – molecule, molecule – molecule reactions-semiconductor catalysis-Homogeneous Catalysis- acid base and redox catalysis.

UNIT – III

Correlation of rate with H_o, H_R, acidity functions and their use in the illustration of mechanism in acid base catalysis – catalysis by transition metal ions and their complexes – Industrially important processes – electron transfer reactions – Marcus theory – Application – substitution reaction in Octahedral complexes.

UNIT – IV

Physical-organic chemistry-Linear free energy relationships for substituent effects.Hammett equation, Taft equation (numerical expression and application to characterization of reaction mechanisms).Chemical bonding in poly atomic molecules- Hybrid orbitals – Qualitative applications -Huckel theory of linear conjugated systems – 1,3 Butadiene and cyclic conjugated molecules- cyclo Butadiene Aromaticity-Calculations of delocalization energy of simple conjugated systems- Benzene .Aromaticity for annulenes – Napthalene, charged rings – cyclopentadienylcation.

UNIT-V

Thermodynamics and kinetics: Acids and bases, HSAB principle, bond energies and thermochemistry, kinetic parameters, Hammond's postulate, Kinetic isotope effects, kinetic and thermodynamic control (general relationship between thermodynamic stability and reaction rate).

Suggested Books:

1. Chemical kinetics by K.J. Laidler
2. Physical Organic Chemistry by Wiberg
3. Physical Organic Chemistry by Neil isaacs
4. Physical basis of Organic Chemistry by Howard Maskul, oxford university press
5. Techniques in Organic Reaction Mechanism by Zuman and Patel.
6. Chemical kinetics – The study of Reaction Rates in solution – Kenneth A. CONNORS – VCH Publishers.
7. Fundamentals of photochemistry – K. K. Rohatgi – Mukherjee
8. Photochemistry – cox and kemp
9. Photochemistry – Calvert by Pitts,

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZATION
FOURTH SEMESTER
PAPER-II QUANTUM CHEMISTRY-III, NUMERICAL METHODS FOR CHEMISTS AND ADVANCED COMPUTER PROGRAMMING
(With effect from the Admitted batch of 2021-2022 Academic Year)

Course Outcomes (COs)-Course Specific Outcomes (CSOs):
Upon completion of the course the students will be able to,
CO1: Solve various problems of approximation methods
CO2: Understand the concepts of VB, MO theories its applications in quantum chemistry.
CO3: Make use of the basic concepts numerical methods
CO4: Explain the Numerical techniques of solving first order differential equations
CO5: Explain the different chemical applications using FORTRAN program.

Learning Outcomes (LOs):
Upon completion of the course the student will be able to
- Use different approximation methods for various applications.
- Apply the knowledge of quantum chemistry in chemical bonding
- Use numerical methods in chemistry.
- Write FORTRAN program for problems in chemistry

CO-PO MAPPING

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	✔	✔	✔		✔	✔	✔	✔
CO2	✔	✔	✔		✔	✔	✔	✔
CO3	✔	✔	✔		✔	✔	✔	✔
CO4	✔	✔	✔		✔	✔	✔	✔
CO5	✔	✔	✔		✔	✔	✔	✔

COURSE CONTENT

UNIT – I
Perturbation theory- time dependent perturbation- First and second order approximations- First order perturbation for degenerate states- Calculation of first and second order perturbation effects onhydrogen atom, excited state hydrogen atom and harmonic oscillator. Time dependent perturbations- Stark effect-Zeeman effect-Derivation of Fermi's Golden rule.

UNIT – II

Hartee-Fockself consistent field method- Calculation of orbital energies for hydrogen and helium atoms-Slater type orbitals.Chemical bonding (diatomic molecules)-Born- Oppenheimer approximation- The LCAO-MO approximation-application to H_2^+ ion – Calculation of energy,
electron density and bonding-Limitations of MO theory- Valence Bond theory-application to H_2^+ ion.

UNIT – III

Numerical Methods-Precision and Accuracy, Determinate and indeterminate errors, computational errors truncation and rounding off errors, algorithm errors-absolute and relative errors-Error propagation.Measures of Dispersion – range, arithmetic mean, mean deviation variance and standard deviation – moments – skewness and kurtosis.Interpolation: interpolation for linear fit, linear interpolation in non-linear fit, polynomial interpolation – Lagrange interpolation formula – Application to complex equilibria.

UNIT-IV

Numerical techniques of solving ordinary first order differential equations:- Euler's method, Predictor-corrector method, RungaeKutta method-application to chemical kinetics.
Fortran programming: Concepts of Alogrithms and flow-charts, logical variables and logical expressions, order of evaluation of logical expressions, logical assignment statements, logical if and block if statements.

UNIT-V

Computed GO TOstatement, writing a decision, chain of decisions, arrays-one dimensional and two dimensional arrays. DO loop and its application in Input and Output statements. Statement Function, Function and Subroutine sub-programs.

Application to Chemical Problems-Flowcharts and Programs for

1. Calculation of skewness and kurtosis of replicate measurements.
2. Polynomial interpolation using Lagrange interpolation formula
3. Euler's step by step iteration method for solving ordinary first order differential equation.
4. Calculation of first order rate constant of acid catalyzed hydrolysis an ester, using a subprogram for the calculation of slope by linear least-squares method.

RECOMMENDED TEXT BOOKS:

11. I.N. Levine, Quantum Chemistry, 5 th edition (2000), Pearson Educ. Inc., New Delhi.
12. D.A. McQuarrie and J.D. Simon, Physical Chemistry: A Molecular Approach, (1998) Viva Books, New Delhi.
13. A.K. Chandra, Introductory Quantum Chemistry, 4 th edition (1994), Tata McGraw Hill, New Delhi.
14. Numerical analysis and computational programming, S. A. Mollah, Books and allied (P) Ltd.
15. R. K. Prasad, Quantum Chemistry, 3rd Ed., New Age International Publishers, 2006.
16. Theoretical Chemistry, S. Glastone
17. Computer programming in Fortran-IV by V .Rajaraman, Prentice-Hall of India Pvt. Ltd., New Delhi.

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZATION
FOURTH SEMESTER
PAPER-III ADVANCED THERMODYNAMICS AND BIOPHYSICAL CHEMISTRY
(With effect from the Admitted batch of 2021-2022 Academic Year)

Course Outcomes (COs)-Course Specific Outcomes (CSOs):
Upon completion of the course the students will be able to,
CO1: Understand the structures of protein and its determination
CO2: Understand basic concepts of forces in protein folding and thermodynamics of protein folding
CO3: Make use of the concepts of thermodynamics and phase equilibrium curves.
CO4: Understand the concepts of entropy production and flow in non-equilibrium thermodynamics
CO5: Understand the applications of thermodynamics of living systems

Learning Outcomes (LOs):
Upon completion of the course the student will be able to
- Understand protein structure and forces in protein folding.
- Use the concepts of thermodynamics in protein folding
- Apply the principles of non-equilibrium thermodynamics and thermodynamics to living systems.
- Determine the structure of protein using various techniques.

CO-PO MAPPING

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	✔	✔			✔	✔	✔	✔
CO2	✔	✔			✔	✔	✔	✔
CO3	✔	✔			✔	✔	✔	✔
CO4	✔	✔			✔	✔	✔	✔
CO5	✔	✔			✔	✔	✔	✔

COURSE CONTENT

UNIT – I

Protein structure- Primary structure of protein - secondary structure of protein - Tertiary structure of protein- Spectroscopic determination –Franck Condon principle- Electronic Spectroscopy-Absorption and fluorescence- Infrared spectroscopy of proteins.

UNIT – II

Forces in protein folding –Intermolecular interaction- Dipole- Dipole interactions – Hydrogen Bonding - Electrostatic forces –Hydrophobic effect- Protein denaturation- Protein floding pathway- Diffusion-langein equation and Brownian motion - Thermodynamics of protein unfolding.

UNIT – III

Thermodynamics and phase changes –Basic concepts of thermodynamics-First law, Second law and Third law of thermodynamics. Free energy and meaning of phase changes, calculation of phase equilibrium curves, Pressure as a measure of escaping tendency, one components phase diagrams, two component system, and three component systems.

UNIT – IV

Elementary aspects of non-equilibrium thermodynamics-conservation of mass and energy in close and open systems - Entropy production due to heat flow –Entropy production in chemical reactions Entropy production and flow in open systems-transformation properties of fluxes and forces- principles of microscopic reversibility-Onsager reciprocal relations.

UNIT – V

Thermodynamics of living systems: Simultaneous coupled reactions, coupled reactions and metabolism free energy utilization, free energy utilization in metabolism, citric acid cycle, Terminal oxidation, Chain aerobic metabolism

Suggested Books

1. Richard E.Dickerson , molecular Thermodynamics
2. S. Glasstone, Theoretical Chemistry, Affiliated East–West Press Pvt. Ltd., New Delhi, 1973.
3. S. Glasstone, Thermodynamics for Chemists, Affiliated East–West Press Pvt. Ltd., New Delhi, 1964.
4. Upadhyay and Upadhyay- Biophysical chemistry.
5. P S Kalsi, DrNiveditaMahanta,Biophysical chemistry
6. Puri, Sharma and Pathania, Principles of Physical chemistry.
7. U.N Dash,.A Text Book of Biophysical Chemistry,Macmillan India Ltd
8. Gurtu and Gurtu,Biophysical Chemistry,PragatiPrakashan.
9. C. Kalidas and M. V. Sangaranarayan, Non-Equilibrium Thermodynamics, Principles and Applications, McMillan India Ltd., 2002

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZATION
FOURTH SEMESTER
PAPER-IV SPECTROSCOPY
(With effect from the Admitted batch of 2021-2022 Academic Year)

Course Outcomes (COs)-Course Specific Outcomes (CSOs):

Upon completion of the course the students will be able to,

CO1: Explain the selection rules and applications of Microwave spectroscopy.

CO2: The student will acquire knowledge of the fundamental concepts of Vibrational and rotational spectroscopy.

CO3: Understand basic concepts and detailed applications of NMR and Mossbauer spectroscopy

CO4: Understand the concepts of ESR spectroscopy and X-ray methods.

CO5: Understand the principles of electron spectroscopy

Learning Outcomes (LOs):

Upon completion of the course the student will be able to

- Use basic principles of NMR and IR for structural elucidation of organic compounds
- Acquire knowledge in applications of spectroscopic techniques
- Understand the instrumentation of spectroscopic techniques.
- Apply the principles of PES, Mossbauer to determine the structure of inorganic compounds.

CO-PO MAPPING

CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
CO1	✔	✔			✔	✔	✔	✔
CO2	✔	✔			✔	✔	✔	✔
CO3	✔	✔		✔	✔	✔	✔	✔
CO4	✔	✔			✔	✔	✔	✔
CO5	✔	✔			✔	✔	✔	✔

COURSE CONTENT

UNIT – I

Rotational (Microwave) Spectroscopy – The rotational energies of polyatomic molecules – Rotational selection rules for linear molecules – symmetric top – Asymmetric top molecules – degeneracy of rotational energy levels – The stark effect in molecular rotational spectra – Molecular Rotation – Nuclear spin coupling – Application of Rotation Spectra – Determination of Inter Nuclear distance – Moment of Inertia and Dipole moment.

UNIT – II

Rotation vibration spectra – selection rules and transitions for the rigid rotator – harmonic oscillator model – parallel and perpendicular bands of linear and symmetric top molecules – Raman active fundamental – Criterion for their appearance – Rotational and vibrational Raman and Infrared studies – AB_2, AB_3 type molecules – correlation of infrared and Raman spectra.

UNIT – III

NMR spectroscopy-chemical shifts and shielding- some application of NMR spectra- effect of chemical exchange on spectra- effect of quadrupole interactions on NMR spectra– an elementary study of more common nuclei with spin 1/2 – Carbon-13, Fluorine -19, Phosphorous-31, Silicon- 29. Quadrupolar nuclei-Lithium-6, Boron-11- Nitogen-14.NMR imaging.Basic principles of Mossbauer spectroscopy- Origin of isomer shifts-Quadrupole splitting-hyperfine splitting-Applications in Fe systems.

UNIT -IV

ESR spectroscopy – the resonance condition – anisotropy in g-factor – Theory and applications of ESR method – Crystalline solids – free radicals in solutions – Interpretation of ESR spectra of typical radicals and ion like Mn^{+2}, Cr^{+3}, Cu^{+2} -Hyperfine interactions in the following systems. P-Benzoquinone – (semi) naphthalene radical anion and anthracene radical anion-Zero field splitting-Krammers degeneracy.

X- ray methods- X-ray fluorescence (XRF and X-ray absorption methods and their applications. X-ray diffraction-Bragg's condition-Powder diffraction technique-Single crystal methods-Laue method and rotating crystal method.

UNIT-V

Electron spectroscopy- basic principles of Photo Electron Spectroscopy (PES)-Koopman's theorem and chemical shift- PES of simple molecules like O_2, N_2, F_2, CO. Vibrational structure of PES bands- Electron Spectroscopy for Chemical Analysis (ESCA)- Chemical information from ESCA- Principles and applications of Auger Electron Spectroscopy (AES)-comparison between PES, ESCA and AES.

RECOMMENDED TEXT BOOKS:

1. Molecular Spectroscopy-I. N. Levine, Wiley-Intersceince publication
2. Modern Spectroscopy – J. M. Hollas, John Wiley & Sons
3. Spectroscopy- D. Satyanarayana
4. C. N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th Ed., Tata-McGraw-Hill, 1994.
5. M. L. Gupta, Atomic and Molecular Spectroscopy, New Age International Publishers, 2001.
6. R. Drago, Physical Methods for Chemists, Saunders, Philadelphia, 1992.
7. B. P. Straughan and S. Walker (Eds.), Spectroscopy – Vol 1-3, Chapman and Hall, New York, 1976.

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZATION
FOURTH SEMESTER
PRACTICAL –I : CHEMICAL KINETICS

(With effect from the Admitted batch of 2021-2022 Academic Year)

Course Objectives:

Upon completion of the course the students will be able to,

CO1: To have hands-on experience/practical knowledge in performing Physical chemistry experiments

CO2: Develop skills on handling instruments like potentiometer and spectrophotometer and perform different types of reactions

CO3: Determine Critical micellar concentration of different surfactants.

CO4: Study the kinetics of different oxidation reactions.

CO5: Developed some understanding of the professional and safety responsibilities residing in working with chemical systems.

Learning Outcomes:

At the end of the course, the learners should be able to:

LO1: Develop/practical skills to solve problems in chemistry.

LO2: Extend the principle of Potentiometric titration to different precipitation reactions

LO3: Determine the absorbance using spectrophotometer and finding the unknown concentration

LO4: Apply kinetics to determine order of reactions.

COURSE CONTENT

1. Kinetics of oxidation of oxalic acid by chromic acid.
2. Effect of chloride ion on stability constant of chromic acid

   -oxalic acid complex.
3. Determination of Critical Micellar Concentration (CMC) of sodium dodecyl Sulphate.
4. Iodination of Acetone.

TEXT BOOKS:

1. A Textbook of Practical Physical Chemistry experiment by Gurtu-Grutu

2. Experiment in Physical Chemistry by Carl w.Garland, Joseph w.Nibler, McGraw-Hill

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZATION
FOURTH SEMESTER
PRACTICAL –II: INSTRUMENTAION
(With effect from the Admitted batch of 2021-2022 Academic Year)

Course Objectives:

Upon completion of the course the students will be able to,

CO1: To have hands-on experience/practical knowledge in performing Physical chemistry experiments

CO2: Develop skills on handling instruments like potentiometer and spectrophotometer and perform different types of reactions

CO3: Determine Critical micellar concentration of different surfactants.

CO4: Study the kinetics of different oxidation reactions.

CO5: Developed some understanding of the professional and safety responsibilities residing in working with chemical systems.

Learning Outcomes:

At the end of the course, the learners should be able to:

LO1: Develop/practical skills to solve problems in chemistry.

LO2: Extend the principle of Potentiometric titration to different precipitation reactions

LO3: Determine the absorbance using spectrophotometer and finding the unknown concentration

LO4: Apply kinetics to determine order of reactions.

COURSE CONTENT

1. pH metric titrations of HClvsNaOH.
2. Potentiometric titrations of KClvs $AgNO_3$.
3. Potentiometric titrations of KI vs$AgNO_3$.
4. Potentiometric titrations of KCl + KI vs $AgNO_3$.
5. Simultaneous determination of Mn(VII) & Cr(VI) by Spectrophotometry.
6. Estimation of Mn(II) by spectrophotometry.

TEXT BOOKS:

1. A Textbook of Practical Physical Chemistry experiment by Gurtu-Grutu

2. Experiment in Physical Chemistry by Carl w.Garland, Joseph w.Nibler, McGraw-Hill

MODEL QUESTION PAPER
ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZATION
FOURTH SEMESTER
PAPER-I-ADVANCED CHEMICAL KINETICS AND PHYSICAL-ORGANIC CHEMISTRY
(With effect from the Admitted batch of 2021-2022 Academic Year)

Time: 3 hours **Max. Marks: 80**

ANSWER ALL QUESTIONS (5×16=80)

1. (a) Discuss theories of Unimolecular gas phase reactions.

   (b) Discuss the kinetics of H_2-Br_2reaction.

(or)

2. (a) Discuss the mechanism of parallel reactions and opposing reactions with examples.

   (b) Describe the flow and relaxation technique for fast reactions.

3. (a) Explain Marcus theory of outer sphere reactions.

   (b) Discuss the mechanism of acid-base catalysis.

(or)

4. (a) Discuss effect of dielectric constant on ion-ion and ion-molecule reactions.

   (b) Write a note on Semiconductor catalysis.

5. (a) Explain the mechanism of base hydrolysis in octahedral complexes

   (b) Discuss the mechanism of catalysis by transition metal ions and their complexes.

(or)

6. (a) Explain the mechanism of acid hydrolysis in octahedral complexes

   (b) Discuss correlation of rate with H_O and H_R acidity functions

7. (a) What is meant by Linear free energy relationships.

   (b) Explain Hammett equation and its importance.

(or)

8. (a) Explain the important features of Huckel theory

   (b) How is delocalization energy of 1, 3-butadiene and benzene calculated.

9. (a) Explain HSAB principle with examples

   (b) Write a note on Hammond's postulate.

(or)

10. (a) Explain about kinetic isotope effects on rate of reaction

(b) What is meant by kinetic and thermodynamic control?

MODEL QUESTION PAPER
ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZATION
FOURTH SEMESTER
PAPER-II QUANTUM CHEMISTRY-III, NUMERICAL METHODS FOR CHEMISTS AND ADVANCED COMPUTER PROGRAMMING
(With effect from the Admitted batch of 2021-2022 Academic Year)

Time: 3 hours **Max. Marks: 80**

ANSWER ALL QUESTIONS (5×16=80)

1. (a) Explain how first and second order approximations of perturbation theory of exited state of hydrogen can be calculated
   (b) Derive Fermi's golden rule in quantum mechanics

(Or)

2. (a) Derive the ground state energy of one dimensional harmonic oscillator using perturbation method
   (b)Explain briefly about second order stark effect using quantum mechanics.

3. (a) Write a note on LCAO approximation
   (b)Describe briefly about Born-Oppenheimer approximation

(Or)

4. (a) Discuss the important features of Hartee-Fock self-consistent field method.
   (b)) Explain the important features of VB theory and write its application to H_2^+ ion.

5. (a) What are determinate and indeterminate errors. Describe their origin and methods of minimization.
   (b) Define the term accuracy and precision. How are these measured?

(Or)

6. (a) What is interpolation. Explain Lagrange interpolation formula?
   (b) Write a note on measures of dispersion

7. (a) Explain Euler's method for solving ordinary first order differential equation
   (b) Write the syntax and flowchart for logical If and block If statements

(Or)

8. (a)Explain RungaeKutta method for solving ordinary first order differential equation
   (b) How do you evaluate the order of logical expressions?

9. (a) Give the syntax and flow chart for DO LOOP
   (b) Write the flowchart and FORTRAN program for Calculation of skewness and kurtosis of replicate measurements

(Or)

10. (a)Write the flowchart and FORTRAN program for calculation of first order rate constant of acid catalyzed hydrolysis an ester, using a subprogram for the calculation of slope by linear least-squares method.

(b) Explain briefly about Subroutine sub-programs.

MODEL QUESTION PAPER
ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZATION
FOURTH SEMESTER
PAPER – III-ADVANCED THERMODYNAMICS AND BIOPHYSICAL CHEMISTRY
(With effect from the Admitted batch of 2021-2022 Academic Year)

Time: 3 hours **Max. Marks: 80**

ANSWER ALL QUESTIONS (5×16=80)

1. (a) State and explain Franck Condon principle
   (b) Explain briefly about IR spectroscopy of proteins

(Or)

2. (a) Write a detailed note on primary, secondary and tertiary structure of protein
   (b) Explain briefly about fluorescence of proteins.

3. (a) Explain in detail about Thermodynamics of protein unfolding.
   (b) Describe the different forces in protein folding.

(Or)

4. (a) Write a note on Protein denaturation
   (b) Discuss briefly about Langein equation

5. (a) Explain different phase changes of change in free energy.
   (b) Construct phase diagram of two component system

(Or)

6. (a) Construct the phase diagram of three component system
   (b) State and explain third law of thermodynamics.

7. (a) Explain in detail the production of entropy and its flow in open systems
   (b)Explain Onsager reciprocal relations.

(Or)

8. (a) Write a brief note on conservation of mass and energy in closed and open systems.
   (b) Explain the principles of microscopic reversibility.

9. (a) Discuss briefly about simultaneous coupled reactions.
   (b)Describe the mechanism of chain aerobic metabolism

(Or)

10. (a) Describe citric acid cycle highlighting energy storing mechanism of living organisms
    (b) What is meant by terminal oxidation?

MODEL QUESTION PAPER
ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
REVISED SYLLABUS FOR PHYSICAL CHEMISTRY SPECILAZTION
FOURTH SEMESTER
PAPER – IV: -MOLECULAR SPECTROSCOPY
(With effect from the Admitted batch of 2021-2022 Academic Year)

Time: 3 hours **Max. Marks: 80**

ANSWER ALL QUESTIONS (5×16=80)

1. (a) Derive an expression for rotational energies of linear polyatomic Molecules
   (b) Discuss the rotational selection rules for symmetric top and asymmetric top molecules.

(or)

2. (a) Discuss the applications of rotational spectra for the determination of moment of inertia and dipole moment.
   (b) Explain the Stark effect in rotational spectroscopy.

3. (a) Describe the parallel and perpendicular bands of linear and symmetric top molecules.
   (b) Discuss the selection rules and transitions for the rigid rotator.

(or)

4. (a) Discuss the rotational and vibrational Raman studies of AB_2, AB_3 type molecules.
   (b) Discuss the Infrared studies of AB_2, AB_3type molecules.

5. (a) Discuss basic principle of Mossbauer spectroscopy and explain origin of isomer shifts.
   (b) Explain quadrupole splitting and hyperfine splitting in Mossbauer spectroscopy

(or)

6. (a) Write the Principle and instrumentation of NMR spectroscopy.
   (b) Explain effect of quadrupole interactions on NMR spectra.

7. (a) What are the factors effecting g-factor in ESR spectroscopy.
   (b) Discuss interpretation of ESR spectra of hydrogen radical, methyl radical and Cu^{2+} ion.

(or)

8. (a) Discuss X-ray fluorescence and X-ray absorption methods and their applications.
   (b) Write a note on Powder diffraction technique.

9. (a) Define basic principle of Photo electron spectroscopy and discuss PES of simple molecules like O_2, N_2 and CO.
   (b) Explain Koopmans's theorem in photo electron spectroscopy.

(or)

10. (a) Discuss principle and applications of Auger electron spectroscopy.
    (b) Give a comparison between PES, ESCA and AES techniques