M.Sc. PHYSICALCHEMISTRY SYLLABUS

FACULTY OF SCIENCE

DEPARTMENT OF CHEMISTRY

SATAVAHANA UNIVERSITY-KARIMNAGAR

UNDER CHOICE BASED CREDIT SYSTEM (CBCS)

DEPARTMENT OF CHEMISTRY

SATAVAHANA UNIVERSITY - KARIMNAGAR

M.SC., CHEMISTRY

Under Choice Based Credit System (CBCS)

SU - M.Sc., (CHE) II SEMESTER

Paper Code	Title	Workload Per Week		Marks			Credits	Duration of the Exams.
		Theory	Practical	Internal	University	Total		
MCHE 201T	Inorganic Chemistry-II	4	--	20	80	100	4	3 Hrs
MCHE 202T	Organic Chemistry-II	4	--	20	80	100	4	3 Hrs
MCHE 203T	Physical Chemistry-II	4	--	20	80	100	4	3 Hrs
MCHE 204T	Analytical Techniques & Spectroscopy-II	4	--	20	80	100	4	3 Hrs
MCHE 205P	Inorganic Chemistry LAB-II	--	6	15	60	75	3	4 Hrs
MCHE 206P	Organic Chemistry LAB-II	--	6	15	60	75	3	4 Hrs
MCHE 207P	Physical Chemistry LAB-II	--	6	15	60	75	3	4 Hrs
MFC* 201T	Fundamentals on Computers & Office Automation	2	--	10	40	50	2	2 Hrs
TOTAL		18	18	135	540	675	27	

***Every student must pass this paper since it is mandatory. However the credits will not included in the calculation of SGPA and CGPA**

CHAIRMAN
Board of Studies in Chemistry
SATAVAHANA UNIVERSITY
KARIMNAGAR- 505 001.

M.Sc. CHEMISTRY SYLLABUS
SEMESTER- II
(Effective from the academic year 2016-2017 for University and affiliated colleges)

Paper CH 103T (PHYSICAL CHEMISTRY)

PC-05: Thermodynamics-II & Statistical Thermodynamics
PC-06: Photochemistry-I
PC-07: Quantum Chemistry-II
PC-08: Solid state chemistry

PC-05: Thermodynamics-II & Statistical Thermodynamics **15 hrs**

Ideal solutions. Thermodynamic properties of ideal solutions. Mixing quantities. Vapour pressure -Raoult's law. Thermodynamic properties of ideally dilute solutions. Vapour pressure- Henry's law. Nonideal systems. Concept of fugacity, fugacity coefficeient. Determination of fugacity. Non ideal solutions. Activities and activity coefficients. Standard-state conventions for non ideal solutions. Determination of activity coefficients from vapour pressure measurements. Activity coefficients of nonvolatile solutes using Gibbs-Duhem equation.

Statistical Thermodynamics: Partition Functions: Concepts of distribution and probability, Boltzmann distribution law. Interpretation of partition functions- translational, rotational, vibrational and electronic partition functions. Relationship between partition functions and thermodynamic functions (only S & G).

PC-06: Photochemistry –I **15 hrs**

Electronic transitions in molecules. The Franck Condon principle. Electronically excited molecules- singlet and triplet states. Radiative life times of excited states-theoretical treatment. Measured life times. Quantum yield and its determination. Experimental set up of a photochemical reaction. Actinometry-ferrioxalate and uranyl oxalate actinometers – problems. Derivation of fluorescence and phosphorescence quantum yields. E-type delayed fluorescence- evaluation of triplet energy splitting(ΔEST). Photophysical processesphotophysical kinetics of unimolecular reactions. Calculation of rate constants of various photophysical processes-problems, State diagrams Photochemical primary processes. Types of photochemical reactions- electron transfer, photodissociation, addition, abstraction, oxidation and isomerization reactions with examples. Effect of light intensity on the rates of photochemical reactions. Photosensitization. Quenching-Stern-Volmer equation. Introduction to fast reactions- Principle of flash photolysis.

PC-07: Quantum chemistry-II **15 hrs**

Cartesian, Polar and spherical polar coordinates and their interrelations.

Schrodinger equation for the hydrogen atom- separation into three equations. Hydrogen like wave functions. Radial and angular functions. Quantum numbers n, l and m and their importance. The radial distribution functions. Hydrogen like orbitals and their representation. Polar plots, contour pots and boundary diagrams.

Many electron systems. Approximate methods. The variation method-variation theorem and its proof. Trial variation function and variation integral. Examples of variational calculations. Paricle in a box. Construction of trial function by the method of linear combinations. Variation parameters. Secular equations and secular determinant.

Bonding in molecules. Molecular orbital theory-basic ideas. Construction of MOs by LCAO, H_2^+ ion. The variationan integral for H_2^+ ion. Detailed calculation of Wave functions and energies for the bonding and antibonding MOs. Physical picture of bonding and antibonding wave functions. Energy diagram. The MO

CHAIRMAN
Board of Studies in Chemistry
SATAVAHANA UNIVERSITY
KARIMNAGAR-505-001.

wave function and the energy of H_2 molecule MO by LCAO method and Valence bond method (detailed calculations not required)-comparison of MO and VB models.

PC-08: Solid state chemistry **15 Hrs**

Electronic properties of metals, insulators and semi-conductors: Electronic structure of solids, Band theory, band structure of metals, insulators and semi-conductors. Electrons, holes and Excitons. The temperature dependence of conductivity of extrinsic semi-conductors. Photo conductivity and photovoltaic effect – p-n junctions. Superconductivity: Occurrence of superconductivity. Destruction of superconductivity by magnetic fields – Meissner effect. Types of superconductors. Theories of super conductivity – BCS theory.

High temperature superconductors: Structure of defect perovskites. High Tc superconductivity in cuprates. Phase diagram of Y-Ba-Cu-O system. Crystal structure of $YBa_2Cu_3O_{7-x}$. Prepartion of 1-2-3 materials. Origin of high Tc superconductivity. **Nanoparticles and their applications:** Introduction to nanoparticles. Reduced dimensionality in solids – zero dimensional systems, fullerenes, quantum dots. One dimensional systems, carbon nano tubes, preparation of nano particles –top down and bottom up methods. Preparation of nanomaterials- – sol gel methods, and chemical vapour deposition method; thermolysis. Applications of nanoparticles.

References:

1. Atkin's Physical Chemistry, Peter Atkins and Julio de Paula, Oxford University press
2. Physical Chemistry, Ira N. Levine, McGraw Hill
3. Physical Chemistry-A Molecular approach, D.A. McQuarrie and J.D. Simon, Viva Books Pvt Ltd
4. Molecular Thermodynamics, D.A. McQuarrie and J.D. Simon, University Science Books
5. Quantum Chemistry, Ira N. Levine, Prentice Hall
6. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill
7. Introduction to Solids, Leonid V. Azaroff, Tata McGraw Hill
8. Solid state Chemistry, D.K. Chakrabarthy, New Age International
9. Solid state Chemistry and its aplications, A.R. West, Plenum.
10. Fundamentals of Photochemistry, K.K.Rohtagi-Mukherji, Wiley-Eastern
11. Molecular Photochemistry, N.J. Turro, Benjamin
12. Photochemistry, R.P.Kundall and A. Gilbert, Thomson Nelson
13. Essentials of Molecular Photochemistry by A. Gilbert and J. Baggott, Blackwell Scientific Publications.
14. Organic Photochemistry by J.M.Coxon and B.Halton, Cambridge University press.
15. Introductory Photochemistry by A.Cox and T.J.Kemp. McGraw-Hill, London.
16. Principles of the Solid State, H. V. Keer, New Age International
17. Elements of Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press
18. Elements of Statistical Thermodynamics, L. K. Nash, Addison – Wesley
19. Introduction to Statistical Thermodynamics, T. L. Hill, Addison Wiley
20. Statistical Thermodynamics, M. C. Gupta, New Age International
21. Quantum Chemistry, D.A. McQuarrie, Prentice Hall
22. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill.
23. Nanostructured Materials and Nanotechnology, edited by Hari Singh Nalwa, Academic Press
24. Self-Assembled Nanostructures, Jin Zhang, Zhong-lin Wang, Jun Liu, Shaowei Chen & Gan-Yu-Liu, Kluwer Academic/Plenum
25. Introduction to Nanotechnology, Charles P. Poole Jr, F. J. Owens, Wiley India Pvt. Ltd.
26. The physics and chemistry of solids by Stephen Elliott, Wiley Publishers.
27. Introductory Photochemistry by A.Cox and T.J.Kemp. McGraw-Hill, London.

CHAIRMAN
Board of Studies in Chemistry
SATAVAHANA UNIVERSITY
KARIMNAGAR- 505 001.

Paper-IV: CH 204T (ANALYTICAL TECHNIQUES AND SPECTROSCOPY-II)

ASP-05: Electro analytical Techniques
ASP-06: NMR- II
ASP-07: Mass Spectroscopy
ASP-08: Electron Spin Resonance (ESR)

ASP-05: Electro Analytical Techniques: (15Hrs)

a) Types and Classification of Electro analytical Methods.

i) Potentiometry- Types of electrodes, Hydrogen gas, Calomel, Quin hydrone and glass electrodes. Determination of P^H. Potentiometric titrations.

ii) Conductometry – Definition of terms – conductivity, specific conductivity, cell constant. Mobility of ions, Conductometric titrations.

b) D.C Polarography: Dropping mercury electrode- Instrumentation-polarogram. Types of Currents: Residual, Migration, Limiting. Two and Three electrode assemblies. Ilkovic equation (derivation not necessary) and its consequences Types of limiting Currents: Adsorption, Diffusion, Kinetic.

Applications of polarography in qualitative and quantitative analysis. Analysis of mixtures. Application to inorganic and organic compounds. Determination of stability constants of complexes.

c) Brief account of following techniques and their advantages over conventional d.c.polargraphy. (i) A.C.polarography (ii) Square-wave polarography (iii) Pulse polarography (iv) Differential pulse polarography

d) Amperometric titrations: Principle, Instrumentation. Types and applications of amperometric titrations. Determination of SO_4^{2-}, metal ions viz., Mg^{2+}, Zn^{2+}, Cu^{2+} and other substances.

e) Cyclic Voltammetry: Principle, instrumentation, reversible and irreversible cyclic voltammograms. Applications. Cyclic voltammetric study of insecticide parathion.

ASP 06: NMR -II: (15Hrs)

^{13}C NMR spectroscopy: Introduction of ^{13}C NMR spectroscopy, types of ^{13}C NMR spectra: undecoupled, proton- decoupled, single frequency off-resonance decoupled (SFORD) and selectively decoupled spectra. ^{13}C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear (^{13}C-^{13}C J) and heteronuclear (^{13}C-^{1}H J , ^{13}C-^{2}H J and ^{13}C-^{19}F J) couplings.
Applications of ^{13}C-NMR spectroscopy: Structure determination, stereochemistry and reaction mechanisms in organic molecules. Principle and applications of DEPT method.

CHAIRMAN
Board of Studies in Chemistry
SATAVAHANA UNIVERSITY
KARIMNAGAR- 505 001.

^{19}F NMR spectroscopy: ^{19}F chemical shifts, coupling constants. Applications of ^{19}F NMR involving coupling with ^{19}F, ^{1}H and ^{31}P: CH_3CHFBr, BrF_5, SF_4, PF_5, ClF_3, IF_5, HF_2^- .
^{31}P NMR spectroscopy: ^{31}P chemical shifts, coupling constants. Applications of ^{31}P NMR involving coupling with ^{31}P , ^{19}F, ^{1}H and ^{13}C: ATP, Ph_3PSe, P_4S_3, $P(OCH_3)_3$, H_3PO_4, H_3PO_3, H_3PO_2, HPF_2, PF_6^-, PH_3,[Rh $(PPh_3)Cl_3$] Rh I=1/2

ASP 07: Mass spectrometry: (15Hrs)

Origin of mass spectrum, principles of EI mass spectrometer. Types of fragments: odd electron and even electron containing neutral and charged species (even electron rule), Nitrogen rule, isotopic peaks, determination of molecular formula, metastable ion peaks. High resolution mass spectrometry. Salient features of fragmentation pattern of organic compounds including β-cleavage, Mclafferty rearrangement, retro Diels – Alder fragmentation and ortho effect. Principle of EI, CI, Fast Atom Bombardment (FAB),Secondary Ion Mass Spectrometry (SIMS), Electrospray (ESI) ionization and Matrix Assisted Laser Desorption Ionization (MALDI) methods. Introduction to principle and applications of Gas Chromatography-Mass Spectrometry (GC-MS) and Liquid chromatography-Mass Spectrometry (LC-MS) techniques.

ASP-08: Electron Spin Resonance: (15Hrs)

Introduction, principle, instrumentation, selection rules, interpretation of Lande's factor 'g'. Hype rfine and super hyperfine Coupling. Anisotropy in 'g' values and hyperfine coupling constants. Zero field splitting, Kramer's degeneracy, quadrupolar interactions. Application of ESR to the study of simple free radicals:

methyl (CH_3), ethyl(C_2H_5), 1,4-benzosemiquinone and naphthalene anion, amine $(NH_2)^{\cdot}$, diphenyl picryl hydrazyl, cyclopentadienyl $(C_5H_5)^{\cdot}$, hydroxy methyl$(CH_2OH)^{\cdot}$ radicals.

Study of free radicals and transition metal complexes. Applications of ESR to Metal Complexes - ESR Spectra of d^1-d^9 Transition Metal Complexes with examples. Interpretation of g in cubic , axial and rhombohedral geometries. Factors affecting g values. Calculation of g values with simple examples. Interpretation of 'g' and 'A' values from esr spect ral data in- i) MnF_6^{4-}, ii) CoF_6^{4-}, and CrF_6^{3-}.

CHAIRMAN
Board of Studies in Chemistry
SATAVAHANA UNIVERSITY
KARIMNAGAR- 505 001.

References:

1. Spectroscopic identification of organic compounds by R.M. Silverstein and F.X. Webster.

2. Organic spectroscopy by William Kemp

3. Mass Spectrometry for Chemists and biochemists by M. Rose and R.A. W. Johnstone

4. Spectroscopic methods in organic chemistry by D.H. Williams and I. Fleming

5. Practical Pharmaceutical Chemistry by A. H. Beckett and J.B. Stenlake

6. Biological Mass Spectrometry by A.L. Burlingame

7. Principles and Practice of Biological Mass Spectrometry by Chhabil Das

8. Spectrscopic identification of organic compounds by R.M.Silverstein.
G.C.Bassler and T.E.Morrill

9. NMR-A multinuclear introduction by William Kemp

10. Stereochemistry of Carbon compounds by Ernest L Eliel / Samuel H. Wilen

11. Principles of Polarography, Heyrovsky.

12. Principles of Polarography, Kapoor.

13. Modern Electroanalytical methods, edited by C.Charlot, Elsevier Company.

14. Principles of Instyrumental analysis, Skoog, Holler and Nieman, Harcourt Asia PTE Ltd.

15. Analytical Chemistry-An Introduction, Skoog, West, Holler and
Crouch, Saunders College Publishing.

16. Prinicples of Instrumental Analysis, Skoog and Leary, Saunders College Publishing.

17. International series of Monographs, Vol. **53**: Photoelectron Spectroscopy,
Edited by D. Beckerand D. Betteridge 1972.

18. Sructural methods in inorganic chemistry, E.A.V. Ebsworth.

CHAIRMAN
Board of Studies in Chemistry
SATAVAHANA UNIVERSITY
KARIMNAGAR- 505 001.