1. Structure of the Programme:

Curriculum Framework
Syllabus – M.Sc. (Chemistry) 2022-23
L-8 (I & II Semester)

I-Semester

Level / Semester	Nature of Course	Courses Code	Course Title	MM	L	T	P	C
L-8	Discipline Specific: Major	CHE-DSM-121	Inorganic Chemistry	100	4	0	0	4
	Discipline Specific: Major	CHE-DSM-122	Laboratory Course: Inorganic Chemistry	100	0	0	2	2
I Semester	Discipline Specific: Major	CHE-DSM-123	Organic Chemistry	100	4	0	0	4
	Discipline Specific: Major	CHE-DSM-124 CHE-DSM-124	Laboratory Course: Organic Chemistry	100	0	0	2	2
	Multi Discipline Major	CHE-MDM-121	Chemical Physics	100	4	0	0	4
	Multi Discipline Major	CHE-MDM-122	Laboratory Course: Chemical Physics	100	0	0	2	2
	Skill Enhancement Course	CHE-SEC-121	Spectroscopy	100	3	0	0	3
	Skill Enhancement Course	CHE-SEC-122	Laboratory Course: Spectroscopy	100	0	0	1	1
Total Credits								**22**

II-Semester

Level / Semester	Nature of Course	Courses Code	Course Title	MM	L	T	P	C
L-5	Discipline Specific: Major	CHE-DSM-221	Inorganic Chemistry	100	4	0	0	4
	Discipline Specific: Major	CHE-DSM-222	Laboratory Course: Inorganic Chemistry	100	0	0	2	2
	Discipline Specific: Major	CHE-DSM-223	Organic Chemistry	100	4	0	0	4
II Semester	Discipline Specific: Major	CHE-DSM-224	Laboratory Course: Organic Chemistry	100	0	0	2	2
	Multi Discipline Major	CHE-MDM-221	Chemical Physics (Theory)	100	4	0	0	4
	Multi Discipline Major	CHE-MDM-222	Laboratory Course: Chemical Physics	100	0	0	2	2
	Skill Enhancement Course	CHE-SEC-221	Computer for Chemist	100	3	0	0	3
	Skill Enhancement Course	CHE-SEC-222 CHE-SEC-222	Computer for Chemist (Laboratory)	100	0	0	1	1
Total Credits								**22**
Exit with Post-Graduate Diploma								

BOS

School Board

Department of Chemistry
Dr. HarisinghGourVishwavidyalaya, Sagar
Scheme of M.Sc. Program in Chemistry under CBCS system
Objectives and Learning Outcomes of M.Sc. Chemistry
(Semester-II)

Department of Chemistry						
Class	**Subject**	**Semester**	**Course Code**	**Course Title**	**Marks**	**Credit**
M.Sc.	Chemistry	Second	CHE-DSM-221	Inorganic Chemistry	100	04

Course Objectives: To impart mechanistic knowledge behind inorganic chemical reactions and processes

Course Learning Outcomes: Upon successful learning, students will be able to
Unit I: access thermodynamic and kinetic knowledge of inorganic reactions
Unit II: be aware of reaction mechanism of nucleophilic substitution and electron transfer reactions of coordination compounds
Unit III: understand chemistry of metal-clusters
Unit IV: investigate the spectral characteristics of electronic transitons
Unit V: apply spectral and magnetic properties of molecule in molecular characterization.

BOS

School Board

M.Sc. Chemistry
CHE-DSM-221 : Inorganic Chemistry
Semester - II

Credits :4 60 Hrs

UNIT I	Reaction Mechanism of Transition Metal Complexes, Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories, the kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidence in favor of conjugate mechanism, anation reactions, reactions without metal-ligand bond cleavage.	12
UNIT II	Substitution reactions in square planer complexes, the trans effect, mechanism of the substitution reaction; Redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer-sphere type reactions, cross-reactions, and Marcus-Hush theory, inner sphere-type reactions.	12
UNIT III	Metal Clusters – Higher Boranes, Carboranes, metalloboranes and metallocarboranes, metal clusters (carbonyl and halide) and compounds with metal-metal multiple bonds (Binuclear and trinuclear). Molecular Recognition and Supramolecular chemistry-Basic concepts, reactivity and catalysis; Interlocked macromolecules: catenanes, rotaxanes, pseudorotaxanes.	12
UNIT IV	Electronic Spectra and Magnetic Properties of Transition Metal complexes Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano energy diagrams for transition metal complexes (d1to d9 states) Calculations of Dq. B, beta &Racah parameters, Charge transfer spectra-(LMCT) and (MLCT).	12
UNIT V	Spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereo-chemical information. Molecular Magnetism: Ferromagnetic &Antiferromagnetic exchange interactions; Neel and Curie Temperature, Magnetic Susceptibility. Anomalous magnetic moments, magnetic exchange coupling, and spin crossover; Exchange Coupled Dinuclear and Trinuclear Compounds.	12

References:

1. J.E.Huheey, Inorganic Chemistry, 4th Ed. Pearson.
2. G.L. Missler and D.A. Tarr, Inorganic Chemistry, 5th Ed., Pearson.
3. B.R. Puri, L.R. Sharma and K.C. Kalia, Principles in Inorganic Chemistry, 34th Ed. Vishal Publishing Co.
4. E.I. Solomon and A.B.P. Lever, Inorganic Electronic Structure and spectroscopy, Wiley
5. R.L.Carlin, Magnetochemistry, Springer Verlag.
6. D.Banerjee, Coordination Chemistry, TMH,N.Delhi,1995
7. M.Satake, Coordination Chemistry, Discovery Publication House New Delhi.
8. D.M.P. Mingos, Essential Trends in Inorganic Chemistry, Oxford Univ. Press, 1995.

BOS

School Board

19-09-2022

Department of Chemistry
Dr. HarisinghGourVishwavidyalaya, Sagar
Scheme of M.Sc. Program in Chemistry under CBCS system
Objectives and Learning Outcomes of M.Sc. Chemistry
(Semester-II)

Department of Chemistry						
Class	**Subject**	**Semester**	**Course Code**	**Course Title**	**Marks**	**Credit**
M.Sc.	Chemistry	Two	CHE-DSM-222	Laboratory Course: Inorganic Chemistry	Mid Sem: 40 End Sem = 60	04

Course Objectives: To impart practical knowledge of synthesis and spectral analysis of molecules

Course Learning Outcomes: Upon successful learning, students will be able to

- Synthesize the inorganic molecules
- Understand spectral characteristics of the molecules
- Apply spectroscopic knowledge in molecular characterization

BoS

School Board

M.Sc. Chemistry, Semester - II
CHE-DSM-222
Laboratory Course – Inorganic Chemitry

Credits :2

Synthesis and Physico-chemical characterization:

(a)Preparation of selected inorganic compounds;

1. $VO(acac)_2$
2. $TiO(C_9H_8NO)_2.2(H_2O)$
3. cis- $K[Cr(C_2O_4)_2(H_2O)_2]$
4. $Na[Cr(NH_3)_2(SCN)_4]$
5. $Mn(acac)_3$
6. $K_3[Fe(C_2O_4)_3]$
7. $Co(NH_3)_6][Co(N)_2)_6]$
8. cis – $[Co(trien)(NO_2]Cl.H_2O$
9. $Hg[Co(SCN)_4]$
10. $[Co(Py)_2Cl_2]$
11. $[Ni(NH)_6)Cl_2$
12. $Ni(dmg)_2$
13. $[Cu(NH_3)_4]SO_4.H_2O$

(b) **Interpretation/calculations based on pre-recorded spectraof complexes** – electronic (UV-Vis), IR, ESR, Thermograms (TGA),Magnetic and electrochemical behaviour.

References

1. W. L. Jolly, Synthesis and Characterization of Inorganic compounds, Prentice Hall
2. N. Gerasimchuk and H. Tyukhtenko, Inorganic Synthesis: A manual for laboratory experiments, Cambridge Scholars publishing co.
3. G. Pass and H. Sutcliffe, Practical Inorganic Chemistry, Springer

BOS

School Board

Department of Chemistry
Dr. HarisinghGourVishwavidyalaya, Sagar
Scheme of M.Sc. Program in Chemistry under CBCS system
Objectives and Learning Outcomes of M.Sc. Chemistry
(Semester-II)

Department of Chemistry						
Class	**Subject**	**Semester**	**Course Code**	**Course Title**	**Marks**	**Credit**
M.Sc.	Chemistry	Second	**CHE-DSM-223**	Organic Chemistry	100	04

Course Objectives: To impart advanced knowledge of reactive intermediates, stereochemistry of organic compounds, pericyclic reactions

Course Learning Outcomes: Upon successful learning, students will be able to learn
Unit-I : The chemistry of different types of aliphatic substitution reaction and its application.
Unit-II : The chemistry of different types of aromatic electrophilic and nucleophilicsubstitution reaction and its application in advanced organic chemistry.
Unit-III : A concept of stereochemistry with stereo chemical aspects of organic synthesis at advance level.
Unit-IV: The mechanistic facets of Addition of Carbon- Carbon multiple bonds and Elimination reactions.
Unit-V : The advance knowledge of Pericyclic Reactions.

BOS

School Board

M.Sc. Chemistry Semester II
Discipline Specific: Major-2
CHE-DSM-223
Organic Chemistry

60 Hrs

Credits: 4

UNIT I. **Aliphatic Electrophilic Substitution** 6

Bimolecular mechanism-S_E2 and S_E1. The S_Ei mechanism, electrophilic substitution accompanied by double bond shifts. Effects of substrates, leaving group and the solvent polarity on the reactivity

UNIT II. **Aromatic Electrophilic Substitution and Nucleophilic substitution** 10

The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, hipso-attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling. Vilsmeir reaction, Gattermann-Koch reaction

The S_NAr, S_N1, benzyne and S_RN1 mechanism. Reactivity-effect of substrate structure, leaving group and attacking nucleophile. The Richter, Sommelet- Hauser and Smiles rearrangements. 15

UNIT III **Stereochemistry**

Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding.

Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereo specific and stereo selective synthesis. Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes,) chirality due to helical shape. Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus. 14

UNIT IV **Addition to Carbon-Carbon Multiple Bonds and Elimination Reactions**

Mechanistic and stereo chemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemo- selectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation.

The E2, E1 and E1CB mechanisms and their spectrum. Orientation of the double bond. Reactivity - effects of substrate structures. Attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination. Claisen and Cope rearrangements. Fluxional tautomerism. Ene reactions. 15

UNIT V. **Pericyclic Reactions** :

Molecular orbital symmetry. Frontier Orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of Pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electro-cyclic reactions- con-rotatory and dis-rotatory motions, 4n, 4n+2 systems, Cycloadditions- antra-facial and supra-facial additions, 4n, 4n+2 systems, 2,2+2 addition of ketenes and 1,3 dipolar cyclo-additions,Sigma tropic rearrangements- suprafacial and antarafacial shifts of H-, sigma tropic shifts involving carbon moieties, 3,3- and 5.5. sigma tropic rearrangements

BOS

School Board

19-09-22

References:

1. Advanced Organic Chemistry-Reactions. Jerry March, John Wile
2. Advanced Organic Chemistry, F.A. Carey and n J.Sundberg, Plenum
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C.K.Ingold, Cornell University Press.
5. Organic Chemistry, R.T. Morrison and R.N.Byd. Prentice Hall.
6. Modern Organic reactions, H.O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M.Coxon, Blackie Academic & Professional
8. Pericyclic Reactions, S.M.Mukherji, Macmillan, India.
9. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P.Singh, Macmillan.
10 Stereochemistry of Organic Compounds D. Nasipuri, New Age International
11 Setereochemistry of Organic Compounds, P.S.Kalsi, New Age International
12 Basic Stereochemistry of Organic Molecules, S.Sengupta, Book, Syndicate Pvt.Ltd. Kolkata, 1987.
13 Organic Photochemistry and Pericyclic Reactions, M.G.Arora, Anmol Publications, N.Delhi, 1994.

BOS

School Board

Department of Chemistry
Dr. HarisinghGourVishwavidyalaya, Sagar
Scheme of M.Sc. Program in Chemistry under CBCS system
Objectives and Learning Outcomes of M.Sc. Chemistry
(Semester-II)

Department of Chemistry						
Class	**Subject**	**Semester**	**Course Code**	**Course Title**	**Marks**	**Credit**
M.Sc.	Chemistry	II	CHE-DSM-224	Laboratory Course - Organic Chemistry	100	02

Course Objectives:

- To develop experimental skills and techniques for organic synthesis and characterization of products by physical and spectral analysis.
- To develop experimental skill for quantitative analysis.

Course Learning Outcomes: Upon successful learning, students will be able to

- To acquire knowledge on principle and different techniques of organic synthesis to prepare various classes of organic compounds and purification methods,
- To gain knowledge on characterization of organic compounds using physical methods and spectroscopic analysis of IR and NMR spectra.
- To understand quantitative analysis and develop experimental skill for determination of number of hydroxyl groups and estimation of amines, phenols in an organic compound using acetylation method.

BOS

School Board

M.Sc. Chemistry Semester II
Discipline Specific: Major-2
CHE-DSM-224
Laboratory Course – Organic Chemistry

Credits:2

Organic Synthesis :
Acetoacetic ester condensation: Synthesis of ethyl n-butylacetonatoacetate.
Cannizziro reaction : 4-Chlorobenzaldehyde as substrate,
Friedel Crafts Reaction;[]-benzoylpropionic acid from succinic anhydride and benzene, Aromatic electrophilic substitutions: Synthesis of p-nitroaniline and p-bromoaniline.
The products may be Characterized by Spectral Techniques.

Quantitative Analysis
Determination of the percentage or number of hydroxyl groups in an organic compound by acetylation method.
Estimation of amines / phenols using bromate solution / or acetylation method

References:

1. D. Pasto, C. Johnson and M. Miller, Experiments and Techniques in Organic Chemistry, Prentice Hall
2. K. L. Williamson, D. C. Heath. Macroscale and Microscale Organic Experiments, 7th Ed, Charles Hartford.
3. H. Middleton, Systematic Qualitative Organic Analysis, H. Middleton, 1939, Adward Arnold/ Digital Library of India.
4. Handbook of Organic Analysis-Qualitative and quantitative, H. Clark, Adward Arnold.
5. Vogel's Textbook of Practical Organic Chemistry, A. R. Tatchell, John Wiley & Sons.

BOS

School Board

14-09-2022

Department of Chemistry
Dr. HarisinghGourVishwavidyalaya, Sagar
Scheme of M.Sc. Program in Chemistry under CBCS system
Objectives and Learning Outcomes of M.Sc. Chemistry
(Semester-II)

Department of Chemistry						
Class	**Subject**	**Semester**	**Course Code**	**Course Title**	**Marks**	**Credit**
M.Sc.	Chemistry	2	CHE-MDM-221	Chemical Physics (Theory) Multi-Disciplinary: Major 3	100	04

Course Objectives: To impart advanced knowledge about quantum mechanics, equilibrium and dynamics of a chemical reaction and different aspects of molecular spectroscopy

Course Learning Outcomes: Upon successful completion of the course, students will be able to understand:

Unit I: Basic principles and laws of Quantum Chemistry
Unit II: Thermodynamics at statistical, molecular and in non-equilibrium states.
Unit III: Dynamics of a chemical reaction.
Unit IV: Understanding various aspects of molecular spectroscopy and rotational spectra
Unit V: Basic principles of vibrational IR, Raman and electronic spectroscopy

BOS

School Board

19-09-2022

M.Sc. Chemistry, Semester - II
Multi-Disciplinary: Major 3 (Theory)
Chemical Physics (CHE-MDM-221)

Credits :4 60 Hrs

UNIT I **Quantum Chemistry :** 12

A Angular Momentum

Ordinary angular momentum, generalized angular momentum, eigenfunctions for angular momentum, eigenvalues of angular momentum, operators using ladder operators, addition of angular moments, spin, antisymmetry and Pauli exclusion principle.

B Electronic Structure of Atoms: Electronic configuration. Russell-Saunders terms and coupling schemes, Slater-Condon parameters, term separation energies of the p^n configuration, term separation energies for the d^n configurations, magnetic effects: spin-orbit coupling and Zeeman splitting introduction to the methods of self consistent field, the virial theorem.

UNIT II **Statistical Thermodynamics**: A.Concept of distribution, thermodynamic and probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and micro canonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). 12

B.Partition functions- translational, rotational, vibrational electronic partition functions, calculation of thermodynamic properties in terms of partition functions. Applications of partition functions.

Heat capacity behaviour of solids- chemical equilibrium constant in terms of partition. Femi-Dirac statistics, distribution law and applications to metal. Bose-Einstein statistics- distribution law and application to helium.

Non Equilibrium Thermodynamics : Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (i.e. heat flow, chemical reaction etc.) fluxes and forces, non equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations, electro-kinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological systems, coupled reactions.

UNIT III **Chemical Dynamics** : A. Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions 12

B) Dynamic chain(hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane). Photochemical(Zhabotinsky reaction). Homogeneous catalysis, kinetics of enzyme reactions, general features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method. Dynamics of molecular motions, probing the transition state, dynamics of barrierless chemical reactions in solution, dynamics of unimolecular reactions (Lindemann- Hinshelwood and Rice-Ramsperger- Kassel-Marcus - RRKM theories of unimolecularreactions).

UNIT IV **Molecular Spectroscopy:** 12

A) Absorption characteristics of organic molecules: electronic transitions and energy levels, molecular orbitals, Frank Condon principle, electronic spectra of polyatomic molecules, emission spectra, radiative and non radiative decay, internal conversion,vibronic transitions, vibrational progression and geometry of the excited states, ultraviolet bands for □□ and □□ bond carbonyl compounds, unsaturated carbonyl compounds, dienes conjugated polyenes,. Fieser Woodward rule (conjugated dienes and carbonyl compounds), uv spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls. effect of solvent on electronic transitions, spectra of transition metal complexes, charge transfer spectra.

B) Rotational Spectra: Di atomic molecules, energy levels of a rigid rotors (semi classicalprinciples), Selection rules, spectral intensity, distribution using population distribution (Maxwell-Boltzmann distribution) determination of bond length, qualitative description of non-rigidrotor, isotope effect

UNIT V A) **Vibrational Spectroscopy : Infrared Spectroscopy and Raman Spectroscopy** 12

Review of linear harmonic oscillator and vibrational energies of di atomic molecules, force constants, overtones, hot bands, Morse potential energy diagrams, vibration-rotation spectroscopy, Zero point energy PQR branches, anharmonicity,breakdown of Oppenhimer approximation. Vibration of poly atomic molecules, selection rules,

BOS School Board

normal modes of vibrations, group frequencies, overtones, hot bands, factors affecting band positions and intensities, far IR region, metal ligand vibrations, normal coordinate analysis.

B) Electronic Spectrum: Concept of potential energy curves for bonding and anti-bonding molecular orbitals, quantitative description of selection rules and Frank Condon principle

References

1. P.W. Atkins, Physical Chemistry; ELBS
2. A.K. Chandra, Introduction to Quantum Chemistry, Tata McGraw Hill,1995
3. Ira N. Levine, Quantum Chemistry, Prentice Hall, 1975
4. Coulson's Valence, R.McWeeny, ELBS.
5. K.J.Laidler, Chemical Kinetics, McGraw Hill.
6. J.Rajaram and J. Kuriacose, Kinetics Mexchanism of Chemical Transformations, McMillan.
7. G.L. Agrawal, Chemical kinetics, TMH, New Delhi
8. R.K. Prasad, Quantum Chemistry, New Age Intl., New delhi.
9. R.P. Rastogi, Introduction to Chemical Thermodynamics, Vikas, Pub. House, New Delhi. 1997.
10. M.C.Gupta, Statistical Thermodynamics, New Age Intl., N.Delhi.
11. Physical Chemistry, G.W. Narosa Publishing House, New Delhi, 1994.

BOS

School Board

19-04-2022

Department of Chemistry
Dr. HarisinghGourVishwavidyalaya, Sagar
Scheme of M.Sc. Program in Chemistry under CBCS system
Objectives and Learning Outcomes of M.Sc. Chemistry
(Semester-II)

Department of Chemistry						
Class	**Subject**	**Semester**	**Course Code**	**Course Title**	**Marks**	**Credit**
M.Sc.	Chemistry	IIndSem	CHE-MDM-222	Chemical Physics:Laboratory Course (Multi-Disciplinary)	Mid Sem: 40 End Sem = 60	02

Course Objectives: To equip the students with the knowledge of various experiments of electrochemistry by using conductometric, potentiometric and pH metric titrations

Course Learning Outcomes:

1. Upon successful learning, students will be able to do investigate conductometric application for the
- Determination of the strength of strong and weak acids in a given solution,
- the effect of solvent on the conductance of $AgNO_3$ /acetic acid
- determination of the degree of dissociation and equilibrium constant in different solventand their mixtures (DMSO, DMF, dioxane, acetone, water)
- the validation of Debye-Huckel-Onsager theory
- determination of the activity coefficient using Debye-Huckel's limiting law

2. Upon successful learning, students will be able to do investigate potentiometric application for the
- determination of the strengths of halides in a mixture
- determination of valency of ions
- determination of the strength of strong acid and weak acids in a given mixture
- investigation of the temperature dependence of EMF of a cell

3. Upon successful learning, students will be able to do investigate **pH metric**application for the
- determination of theactivity and activity coefficient of electrolytes
- determination of thedissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating it with KOH
- determination of the thermodynamic constants ΔG, ΔH, ΔS for the reaction by e.m.f. method

BOS

School Board

M.Sc. Chemistry, Semester – II
Chemical Physics (Laboratory Course)
(CHE-MDM-222)

Credits :2

Instrumental :Electrochemistry*A. Conductometry :*
Determination of the Velocity constant, order of reaction and energy of activation for saponification of ethylacetate by sodium hydroxide conductometrically.
Determination of solubility and solubility product of sparingly soluble salts (e.g. $PbSO_4$, $BaSO_4$) conductometrically.

- Determination of the strength of strong and weak acids in a given solution by conductometry.
- To study the effect of solvent on the conductance of $AgNO_3$ /acetic acid and
- to determine the degree of dissociation and equilibrium constant in different solvents and their mixtures (DMSO, DMF, dioxane, acetone, water) and
- to test the validity of Debye-Huckel-Onsager theory.
- Determination of activity coefficient of Zn ions in the solution of 0.002 M $ZnSO_4$ using Debye-Huckel's limiting law.

B. Potentiometry / pH metry

- Determination of strengths of halides in a mixture potentiometrically.
- Determination of valency of mercurous ions potentiometrically.
- Determination of the strength of strong acid and weak acids in a given mixture using potentiometer / pH meter.
- Determination of the temperature dependence of EMF of a cell.
- Determination of the formation constant of silver-ammonia complex and stoichiometry of the complex potentiometerically.

Acid-base titration in a non-aqueous media using a pH meter.

- Determination of activity and activity coefficient of electrolytes.
- Determination of dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating it with KOH.
- Determination of thermodynamic constants ΔG, ΔH, ΔS for the reaction by e.m.f. method. $Zn + H_2SO_4 \rightarrow ZnSO_4 + 2H$□□

References

1. J.N. Gurtu & A. Gurtu, Advanced Physical Chemistry Experiments, 2011, Pragati Prakashan.
2. J.B. Yadava, Advanced Physical Chemistry, 2015, Krishna Prakashan.
3. Experimental Physical Chemistry, R. C. Das and B. Behera, Tata McGraw Hill.
4. Practical Physical Chemistry, A. M. James and F. E. Prichard, Longman.
5. B. P. Levitt, Findley's Practical Physical Chemistry, Longman.

BOS

School Board

Department of Chemistry
Dr. HarisinghGourVishwavidyalaya, Sagar
Scheme of M.Sc. Program in Chemistry under CBCS system
Objectives and Learning Outcomes of M.Sc. Chemistry
(Semester-II)

Department of Chemistry						
Class	**Subject**	**Semester**	**Course Code**	**Course Title**	**Marks**	**Credit**
M.Sc.	Chemistry	Second	CHE-SEC-221	Computer for Chemist Skill Enhancement Course (Theory)	100	03

Course Objectives: To equip the students with the knowledge of programming in FORTRAN

Course Learning Outcomes: Upon successful learning, students will be able to
Unit I: know the basic structure and functioning of a computer
Unit II: Learns FORTRAN language and various FORTRAN Statements and expressions
Unit III: Develops small FORTRAN code using Chemistry formulas
Unit IV: Develop code for the laboratory data analysis such as linear regression
Unit V: how to operate standard program packages such as MS Excel using PC.

BOS

School Board

Skill Enhancement Courses (Theory) M.Sc. Chemistry, Semester –II CHE-SEC-221: Computer for Chemist		
Credits:03		45 Hrs
UNIT I	**Introduction to computers and computing** Basic structure and functioning of computers with a PC as an illustrative example. Memory, I/O devices. Secondary storage. Computer languages. Operating systems with DOS as an example. Introduction to Unix and Windows, data processing, principles of programming. Algorithms and flow charts.	9
UNIT II	**Computer programming in FORTRAN/ C/ BASIC** (The language features are listed here with respect to FORTRAN. The instructor may choose another language such as BASIC or C and the features may be replaced appropriately). Elements of the computer language. Constants and variables. Operations and symbols. Expression. Arithmetic assignment statement. Input and Output. Format statement. Termination statement. Branching statements such as IF or GO TO statements. LOGICAL variables. Double precision variables. Subscripted variables and DIMENSION. DO statement. FUNCTION and SUBROUTINE. COMMON and DATA statements.(Note: Students learn these programming logics by "hand on" experience on a personnel computer).	9
UNIT III	**Programming in Chemistry** Development of small computer codes involving simple formulae in chemistry, such as van der Waal equation, pH titration, kinetics, radioactive decay. Evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equation to solve secular equation with Huckel theory. Elementary structural features such as bond lengths, bond angles, dihedral angles etc.	9
UNIT IV	Programs with data preferably from physical chemistry laboratory. Execution of linear regression such as X Y plot, numerical integration and differentiation as well as differential equation solution programs. Monte Carlo and molecular dynamics.	9
UNIT V	**Use of Computer Programs:** The students will learn to how to operate a PC and how to run standard programs and packages. Further, the students will operate one or two or more packages such EXCEL,MS Word and Power point.	9

References

1. Computers and Common Sense, R.Hunt and J.Wiley, Prentice Hall.
2. Computational Chemistry, A.C.Norris,
3. Microcomputers Quantum Mechanics, J.P.Lillingbeck, Adam Hilger.
4. Computer Programming in FORTRAN IV,V.Rajaraman, Prentice Hall,
5. An Introduction to Digital Computer Design, V.Rajaraman and T.Radhakrishnan, Prentice Hall.

BOS

School Board

19-09-2021

Department of Chemistry
Dr. HarisinghGourVishwavidyalaya, Sagar
Scheme of M.Sc. Program in Chemistry under CBCS system
Objectives and Learning Outcomes of M.Sc. Chemistry
(Semester-II)

Department of Chemistry						
Class	**Subject**	**Semester**	**Course Code**	**Course Title**	**Marks**	**Credit**
M.Sc.	Chemistry	Second	CHE-SEC-222	Computer for Chemist (Laboratory) Skill Enhancement Course	100	01

Course Objectives: To equip the students with the knowledge of using the standard program packages on computers and do small computer codes using FORTRAN

Course Learning Outcomes: Upon successful learning, students will be able to
Unit I: learn to operate standard program packages such as MS Excel using PC.
Unit II: develop code for linear regression, numerical differentiation etc
Unit III: develop FORTRAN code for the chemistry based formulas
Unit IV: develop code for the laboratory data analysis such as linear regression
Unit V: learn the use of program packages MS word, Excel and power-point etc.

BOS

School Board

Skill Enhancement Courses: (Laboratory)
M.Sc. Chemistry, Semester –II

CHE-SEC-222: Computer for Chemist (Laboratory work)

Credit: 01

The students will learn to how to operate a PC and how to run standard programmer and packages – for chemistry applications.
Execution of linear regression such as X Y plot, numerical integration and differentiation as well as differential equation solution programmer.
Development of small computer codes involving simple formulae in chemistry, – Programming with data preferably from physical chemistry laboratory-Basic/C/Fortran.
Operation of one or two or more packages such as EXCEL, Word Processing software – MS Word and Power point.

References

1. Computers and Common Sense, R.Hunt and J.Wiley, Prentice Hall.
2. Computational Chemistry, A.C.Norris,
3. Microcomputers Quantum Mechanics, J.P.Lillingbeck, Adam Hilger.
4. Computer Programming in FORTRAN IV,V.Rajaraman, Prentice Hall,
5. An Introduction to Digital Computer Design, V.Rajaraman and T.Radhakrishnan, Prentice Hall.

BOS

School Board