DISCIPLINESPECIFICELECTIVECOURSES

.

DISCIPLINESPECIFICELECTIVECOURSE(DSE)

CREDITDISTRIBUTION,ELIGIBILITY,ANDPRE-REQUISITESOFTHECOURSE

Coursetitle&Code	Credits	Creditdistribution of the course			Eligibility criteria	Pre-requisiteof the course (ifany)
		Lecture	Tutorial	Practical		
Supramolecular& Photoinorganic Chemistry **CH-DSE-104**	**04**	**03**	—	**01**	U.G. Chemistry	--

Course objectives

TheObjectivesofthiscourseareas follows:

- Tocomprehendthefundamentalknowledgeofsupramolecularchemistryanditsimportance.
- Toimpartadvancedknowledgethecrystalengineeringandcatalysisofsupramolecular complexes and their applications.
- KnowledgeofvariousPhotochemicalelectrontransferinmetalcomplexesandtheir applications.

Learningoutcomes

Aftercompletingthecourse,the studentswillbeable to:

- Demonstratetheroleofsupramolecularchemistryinunderstandingofmolecular bonding and structure.
- Interpretthesupramolecularinteractionsinproteinsandenzymes.
- Elucidatethe understandingofself-assemblyof biological molecules.
- Understand various types of photochemical reactions of coordination compounds and solar energy conversion in semiconductor systems.

THEORYCOMPONENT **(3Credit.45Hours)**

UNIT1: **(8 Hours)**

FUNDAMENTALSOFSUPRAMOLECULAR CHEMISTRY

Classification of Molecules, Large Molecules, Supermolecules, and Supramolecules, Nomenclature,ThermodynamicandKineticselectivity,Supramolecularinteractions,Chelate, macrocyclic, and macro-bicyclic effects, High dilution synthesis, Template synthesis.

UNIT2: **(15Hours)**

CRYSTALENGINEERING

Introduction to Tectons and Synthons and their classification; Hydrogen bonds, strong, moderate, weak H-bonds; acidity and basicity of hydrogen bonds and hydrogen bonding Synthons; Use of H-bonds in crystal engineering and molecular recognition.

SELF-ASSEMBLY&MOLECULAR RECOGNITION

Introductiontoself-assembly;biologicalexamplesofself-assembly;self-assemblyinsynthetic systems; self-assembly in coordination complexes; Supramolecular host design, Macrocyclic versus acyclic hosts, Catenanes; Rotaxanes.

SUPRAMOLECULARCATALYSIS

Introduction; supramolecular interactions in proteins and enzymes for the control of their function; enzyme mimics; artificial enzymes; supramolecular catalysis in synthetic systems.

UNIT3: **(22 Hours)**

PHOTOINORGANICCHEMISTRY

Introduction to inorganic photochemistry, Redox reactions of transition metal complexes in excited states, excited-state electron transfer, Marcus-Hush model, Photochemical electron transferin$[Ru(bipy)_3]^{2+}$,$[Os(bpy)_3]^{2+}$and$[Fe(bpy)_3]^{3+}$complexes,Roleofspin-orbitcoupling, life-timesofexcitedstatesinthesecomplexes,Photochemicalsupramoleculardevices,devices for photo-induced energy or electron transfer, photo-chemically driven molecular machines.

ENERGYCONVERSION

Solar energy storage, solar energy conversion, Metal complex sensitizers and electron relays insemiconductorsupportedmetaloxidesystems,water-photolysis,NitrogenfixationandCO_2

reduction. Supramolecular photochemistry in natural and artificial systems: photosynthesis, bacterial photosynthesis and artificial photosynthesis.

PRACTICALCOMPONENT **(1Credit:30Hours)**

EXPERIMENTS:

1. Synthesis,characterization(XRD,IR,UV,TGA,etc.)ofsemiconductorsmetal oxides and their photocatalytic applications.
2. SynthesisofaseriesofCr(III)complexes(withligandsofvaryingligandfield strength), electronic spectral interpretation.
3. Synthesis,spectralstudiesandcrystalstructureofRu(II)and Os(II) complexes.
4. Anyother relevant experiment from timeto timeduringthe semester.

ESSENTIAL/RECOMMENDEDREADINGS(Theory)

1. Christian,G.D.,AnalyticalChemistry,6thEd.,JohnWiley&Sons,Inc.(2004).
2. Khopkar,S.M.,BasicConceptsofAnalyticalChemistry3rdEdition,Publisher:NewAge International Publishers (2008), ISBN: 9788122420920, 8122420923.
3. Eldik,R.V.;StochelG.AdvancesinInorganicChemistry:InorganicPhotochemistry,Volume 63, 1st Edition, Academic Press (2011)
4. Hartley,F.R.,Burgess,C.&Alcock,R.M.SolutionEquilibria.Prentice-Hall:Europe(1980).
5. Atwood,J.L.&Steed,J.W.SupramolecularChemistry:AConciseIntroductionJohnWiley & Sons (2000).
6. Lehn,J.M.SupramolecularChemistry:Concepts&Perspectives,Print ISBN:9783527293124 Wiley-VCH (2006).
7. PrinciplesandApplicationsofPhotochemistry,B.Wardle,JohnWiley,2009
8. LigandFieldTheoryandItsApplications;B.A.FiggisandM.A.Hitchman;Wiley India, 2000
9. MechanismofInorganicReactions;Katakis,Gordon;Wiley;1987.
10. InorganicChemistry,Principlesofstructureandreactivity;4thedn;J.E.Huheey,E.A.Keiter and R. L. Keiter. Pearson Education Inc.2003
11. MechanismofInorganicReactions,2ndedn,Basalo,Pearson;WileyEastern,1997.
12. Photochemistry,C.J.WayneandR.P.Wayne;OxfordUniversityPress;1996.

Assessmentmethods:Allexaminationandassessmentsmethodsshallbeinlinewiththe University of Delhi guidelines issued from time to time.

DISCIPLINESPECIFICELECTIVECOURSE(CH-DSE-105)

CREDITDISTRIBUTION,ELIGIBILITY,ANDPRE-REQUISITESOFTHECOURSE

Course title &Code	Credits	Creditdistributionofthe course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Advanced Stereochemistryof Organic Compounds **CH-DSE-105**	**4**	**3**	**0**	**1**	U.G. Chemistry	NIL

Course Objectives: To impart knowledge of advanced concepts of stereochemical principles and asymmetric synthesis of organic compounds, and provide hands-on training in the synthesis and resolution of chiral compounds through laboratory experiments.

Learning Outcomes: Students will develop the ability to analyse the spatial arrangements, and study the properties and reactivity of stereoisomers through the knowledge of symmetry and chirality in organic molecules, gained through this course. The students will be able to predict and design different methods to attain enantioselectivity and diastereoselectivity in a reaction and examine the factors guiding the observed stereoselectivities. Students will attain hands-on training in synthesis, resolution, and optical purity determination of chiral compoundsthroughlaboratoryexperimentsthatwouldenhanceemployabilityinthechemical, especiallypharmaceutical,industrywheresyntheticorganicchemistsworkonstereo-selective synthesis of industrially relevant compounds.

SYLLABUSOFCH-DSE-105

THEORYCOMPONENT **(3Credits.45Hours)**

UNIT1: **(15 Hours)**

MOLECULARSYMMETRYANDCHIRALITY

Symmetry operations and symmetry elements, point group classification, and symmetry number.

STEREOISOMERISM

Classification, racemic modification, molecules with one, two or more chiral centres; Assigningconfiguration(D/L,R/S,E/ZandP/M).Axial,planar,andhelicalchirality;

stereochemistry of allenes, spiranes, alkylidine cycloalkanes, adamantanes, catenanes, biphenyls (atropisomerism), bridged biphenyls, ansa compounds, and cyclophanes.

TOPICITYANDPROSTEREOISOMERISM

Topicity of ligands and faces and their nomenclature; Stereogenicity, chirogenicity, and pseudoasymmetry, stereogenic and prochiral centres. Simple chemical correlation of configurations with examples, quasiracemates.

UNIT2: (15 Hours)

CYCLOSTEREOISOMERISM

Configurations, conformations and stability of cyclohexanes (di-, and trisubstituted), cyclohexenes, cyclohexanones, halocyclohexanones, decalins, decalols and decalones.

MOLECULARDISSYMMETRYANDCHIROPTICALPROPERTIES

Linearand circularlypolarisedlights,circularbirefringenceand circulardichroism,ORDand CDcurves,Cottoneffect.Theaxialhaloketonerule,octantdiagrams,helicity,andLowe'srule. Application of ORD and CD to structural and stereochemical problems.

UNIT3: (15 Hours)

ASYMMETRICINDUCTION

Cram's, Prelog's, and Felkin-Ahn models; Dynamic stereochemistry (acyclic and cyclic), Qualitative correlation between conformation and reactivity, Curtin-Hammett Principle.

ASYMMETRICSYNTHESIS

Significance and basic principles, stereoselective and stereospecific synthesis: Enantioselective and diastereoselective reactions. Methods of asymmetric synthesis: Resolution – Classical resolution, kinetic resolution, and dynamic kinetic resolution of racemic compounds/*meso*-compounds by resolving agents. Development in asymmetric synthesis from prochiral substrates using chiral auxiliaries, chiral reagents, and chiral catalysts.

PRACTICAL COMPONENT (1Credit:30Hours)

EXPERIMENTS

(i) Determinationofopticalpurityoforganiccompoundssuchastartaricacid,glucose, phenylalanine, proline, and limonene etc. by polarimeter.

(ii) Classical resolution of racemic compounds such as cis-/trans-1,2-diaominocyclohexane or 1-phenyl ethylamine by using a resolving agent.

(iii) Synthesisofracemic BINOL.

(iv) Resolution of racemic BINOL using (1*R*,2*R*)-diaminocyclohexane and determination of optical purity by polarimeter.

(v) *cis*-/*trans*-Isomerisationofalkenes.

(vi) Asymmetricaldolreactioncatalysedby(L)-proline/(L)-prolinamide.
(vii) Oxidativekineticresolutionofsecondaryalcoholsbyusing(1*R*,2*R*)-Jacobsen Mn(III) salen complex using an oxidant
(viii) DeterminetheCottoneffectofchiralcompoundsbyCD.

ESSENTIAL/RECOMMENDEDREADINGS

1. Eliel,E.L.StereochemistryofCarbonCompounds,TextbookPublishers(2003).
2. Nasipuri, D.N.StereochemistryofOrganicCompounds: Principles&Applications, South Asia Books (1994).
3. Kalsi,P.S.Stereochemistry:ConformationandMechanism,NewAgeInternational Pvt. Ltd. (2022)
4. Finar,I.L.OrganicChemistryVol.1,Longman(1998).
5. Bruice,P.Y.OrganicChemistry,PearsonEducation,(2020)
6. Sengupta,S.BasicStereochemistryofOrganicMolecules,OxfordUniversityPress (2018)
7. Clayden, J; Greeves, N.; Warren, S. Organic Chemistry, Oxford University Press, (2014)
8. Gawley,R.E.;Aube,J.PrinciplesofAsymmetricSynthesis(Tetrahedronseriesin Organic Chemistry), Pergman, (1996).
9. CatalyticAsymmetricSynthesisI.Ojima,Ed.;VCH:NewYork,(1993).
10. Schanz, H.; Linseis, M. A.; Gilheany, D. G. Improved resolution methods for (R,R)-and(S,S)-cyclohexane-1,2-diamineand(R)-and(S)-Binol.Tetrahedron: Asymmetry, 2003, 14, 2763.
11. Walsh, P. J., Smith, D.K.; Castello, C. Resolution of Trans-Cyclohexane-1,2-diamineandDeterminationoftheEnantiopurityUsingChiralSolidPhaseHPLC Techniques and Polarimetry. J. Chem. Educ. 1998; 75, 11, 1459.

Assessmentmethods: Allexaminationandassessmentsmethodsshallbeinlinewiththe University of Delhi guidelines issued from time to time.

DISCIPLINESPECIFICELECTIVECOURSE(DSE)

CREDITDISTRIBUTION,ELIGIBILITY,ANDPRE-REQUISITESOFTHECOURSE

Coursetitle&Code	Credits	Creditdistributionofthecourse			Eligibility criteria	Pre-requisite of the course (ifany)
		Lecture	Tutorial	Practical /Practice		
Fundamentals of Mathematics for Chemistry **CH-DSE-106**	**04**	**03**	**-**	**01**	U.G. Chemistry	10+2 in Science with Mathematics

Course Objective:

- To develop a sound foundation in mathematical methods essential for basics in study and research of Chemistry.
- Tounderstandtheapplicationoflinearalgebra,multivariablecalculus,differential equations, Fourier and other integral transforms, and statistical methods.
- Tofocusonmathematicalapproachesrelevanttoquantumchemistry,thermodynamics, kinetics, spectroscopy, and data analysis.
- To advance analytical skills to formulate and solve mathematical models of complex chemical systems.
- Topreparestudentstointerpretexperimentaldataquantitativelyandengagein computational and theoretical chemical research.

LearningOutcomes: Bythe endofthiscourse, studentswill beable to:

- Recognizeandapplybasiccalculusconcepts,includingdifferentiationand integration in quantum chemistry, thermodynamics, electrochemistry, and kinetics.
- Solvedifferentialequationsrelevanttophysicalchemistryproblems.
- Understandbasiclinearalgebra,includingvectorsandmatrices,todescribemolecular structures and quantum systems.
- Applyelementarystatistics foranalyzingchemical dataandphenomena.
- Interpret functions of several variables and use partial derivatives in thermodynamics and physical chemistry contexts.

Theory Course Contents: **Credit3(45hours)**

Unit I: **15 hours**

A. OperatorsandEigen-vectors:Linearoperatorandgeometricalinterpretation,Linearvector spaces; linear independence (qualitative discussion on Wronskian), basis vectors, inner product, Dirac bra-ket notation, hermitian conjugates (differential operators). Orthonormal sets. Completeness.

B. Vectors:Differentiationandintegrationofvectors,scalarandvectorfields,divergence&

curl,theoremsonline,surface,andvolumeintegrals.Transformationofrectilinearcartesianto curvilinear spherical polar coordinates.

UnitII: **15 hours**

A. Differential calculus: Ordinary differential equations (ODE), ordinary and singular points of an ODE, and Partial differential equations (PDE), general solution of homogeneous equations. Power series solutions- particle in a box model, solutions ofAssociated Legendre polynomials- for integer *l* and second solution, harmonic oscillator, Laguerre, and associated Laguerre polynomials. Linear ODE of hypergeometric functions (qualitative discussion); Generating functions-recursion formulae and orthonormality: Hermite, Legendre, and Laguerre Polynomials.

B. Determinant and matrices: Properties of determinants and Laplace expansion (qualitative discussion).Matrices- diagonal, symmetricand anti-symmetric, hermitian and anti-hermitian, orthogonal,andunitarymatrices,normalmatrices,EigenvectorsandeigenvaluesofHermitian and unitary matrices, Cayley-Hamilton theorem, degenerate eigenvalues, Diagonalization of matrices (change of basis and similarity transformation).

Unit III: **15 hours**

A. Fourier sine-, cosine-, and exponential series. Fourier transform, Dirac delta function, Fourier sine and cosine transforms, applications of Fourier transforms. Laplace transform, theorems and Inverse Laplace transform, Solution of initial value problems using Laplace transform.

H-atom(quantitativediscussion),Virialtheorem,Hyper-virialtheorem,anditsapplicationsto harmonic oscillator and H-like atoms.

B. Algebra of spin: Stern-Gerlach experiment, concept of spin operators and spin-eigenfunctions, two-electron spin systems; Pauli Exclusion Principle, Hartree product, antisymmetrization operator and Slater determinantal wavefunctions (qualitative discussion). Multiconfiguration calculations and Hartree-Fock theory (qualitative discussion).

RecommendedTexts/References:

1. Pilar F. L. Elementary Quantum Chemistry 2nd Ed., Dover Publication Inc.: N.Y. (2001).

2. Cohen-Tannoudji, Claude, Bernard Diu, and Franck Laloë F., Quantum Mechanics (Translated by G. G. Levine and D. S. Constable), vols-I&II, Wiley-Interscience, New York (1977).

3. Levine, I.L.QuantumChemistry5th Ed.,Prentice-HallInc.:NewJersey(2000).

4. Atkins, Peter, and Ronald Friedman. Molecular Quantum Mechanics, Oxford University Press, 5th ed. (2011).

5. HowardAnton,ElementaryLinearAlgebra,JohnWiley&Sons (2010).

6. Mortimer, Robert G., Mathematics for Physical Chemistry, 3rd ed., Academic Press (2010).

7. Arfken, George B., Hans J. Weber, and Frank E. Harris. Mathematical Methods for Physicists, 7th ed., Academic Press (2012).

8. Kreyszig,E.,Advanced EngineeringMathematics,JohnWiley&Sons, Inc.(2006).

9. Boas,MaryL.,MathematicalMethodsinthePhysicalSciences,3rded.,Wiley (2005).

PracticalComponents **Credit 1**

1. Plotatomicorbitals(SphericalHarmonics$S(\theta)versus\theta$usingpolargraphpaper. Students will be provided with the p-, d-, and f- functions.
2. Plotwavefunctions$\psi_n(x)$,andprobabilitydensities$|\psi_n(x)|^2$forthe1Dharmonic oscillator at different energy levels over the domain $-\infty < x < +\infty$.
3. Calculatethebondlengthofconjugateddyemolecules(e.g.,cyanine, β-carotene,etc.) using the particle-in-a-1D-box model.
4. AssignIRbandsusingsymmetryconsiderationsandselectionrulesforvariousmolecules.
5. Developfamiliaritywith computationaltoolsforanalysisofexperimentaldata:
   (a) Wordprocessing,electronicspreadsheetsetc.
   (b) Dataprocessingsoftware,mathematicalpackages,etc.
   (c) Chemicalstructuredrawing, andmolecularmodelling,etc.
6. Performstatisticaltreatmentoferroranalysis,including:
   (a) Nullhypothesistesting,
   (b) T-test,F-test,Q-test(criteriaforrejectionofhypothesis),
   (c) Statisticalanalysisof laboratorydata.
7. Determine standard deviation, mean and maximum absolute errors, root-mean-square deviation (error), and correlation coefficient of linear straight-line plots.

RecommendedTexts/References:

1. McQuarrie,D.A. &Simon,J.D.*PhysicalChemistry:AMolecularApproach* 3rdEd., Univ. Science Books (2001).
2. Skoog, D. A.; Holler, F. J.; Crouch, S. R. Principles of Instrumental Analysis, Brooks/Cole Pub Co; 7th edition (1 January 2017).
3. Skoog, D. A.; West, D. M.; Holler, F. J.; Crouch, S. R. Fundamentals of Analytical Chemistry,Publisher:Holt,Rinehart&WinstonofCanadaLtd;International2Revised ed edition (1 February 1988).

SKILLENHANCEMENTCOURSES

SKILLENHANCEMENTCOURSE(SEC)

CREDITDISTRIBUTION,ELIGIBILITY,ANDPRE-REQUISITESOFTHECOURSE

Coursetitle&Code	Credits	Creditdistribution of the course			Eligibility criteria	Pre-requisiteof the course (if any)
		Lecture	Tutorial	Practical / Practice		
Introduction to Basic Lab Safety and Softwares for Research work **CH-SEC-107**	**02**	**01**	—	**01**	U.G. Chemistry	--

Course Objectives:

Thecourseisdesignedtoprovidethefundamentalunderstandingoftheprincipleofoperation, interpretationandlearningofchemistryrelatedsoftwaresandSpectralAnalysis,whichwillbe highly helpful especially for their higher studies.

Learning Outcomes:

Thestudentswillbeto:

1. Beawareoftheirandlabsafety.
2. Analyze, interpret and index experimental data/theoretical data collected after various characterizations of their inorganic materials. It will enhance understanding of chemical concepts, improveproblem-solvingskills and theabilityto utilizevarious tools in research and analysis.
3. Understandreactionmechanisms,visualizingmolecularinteractions,quantitativeanalysis, datainterpretation,reportwritingandpresentation,accesstoscientificliteratures,software proficiency etc.

THEORYCOMPONENT **(1Credit:15Hours)**

Unit-I **(15Hours)**

Typesofpersonalprotections(suchaseyeprotection,gloves,labcoats,fireextinguishersetc.) theiruse,andlimitations.Physicalhazardslikefiresafety,electricalsafety,glasswaresafety,

radiation safety etc. Materials Safety Data Sheet (MSDS) file of all the available chemicals. Disposal of chemical waste, handling of hazardous chemicals, Identification of corrosives, flammables, and toxic substances etc. Handling and storing chemicals, including segregation and labelling.

ChemDraw: Widely used for creating 2D and 3D chemical structures, reactions, and pathways.

Origin: Adata analysis and graphing software used for visualizing and analyzing data from experiments.

Chemsketch: To draw chemical structures, such as inorganic, organic, organometallic, polymers etc.

Vesta:A 3Dvisualizationtoolforstructuraldatafiles,includingthosefrom crystallography.Chemical Databases and their utility.

X-pert High-score: Widely used to analyze X-ray diffraction (XRD) data with various applications such as phase identification, crystallographic analysis, cluster analysis, and Rietveld calculations.

International Centre for Diffraction Data (ICDD): Used to identify crystalline phases in materials using X-ray diffraction (XRD) data. It allows researchers to compare experimental XRD patterns against a vast database of reference patterns to determine the composition and structure of unknown materials.

Inorganic Crystal Structure Database (ICSD): To search, visualize, and analyze crystal structures.Valuable software for materials scientists, crystallographers, and other researchers whoneedpreciseinformationaboutthearrangementofatomsinsolids.**ScifinderandWebof**

Science: Databases and search engines for Chemical Literature.

Mendeley: Toorganize,manage,andciteresearchpapers,articles,andothersources.

PRACTICALCOMPONENT (1Credit:30Hours)

EXPERIMENTS:

1. UseofChemDraw tocreate2Dand3D chemical structures.
2. DataanalysisandinterpretationusingOriginfor2Dand3Dgraphs,performingstatistical analysis, signal processing, curve fitting and peak analysis.
3. Drawing,editing,andvisualizingchemicalstructures,reactiondrawing,molecularproperty calculations using Chemsketch software
4. Modeling and visualizing crystal structures,including unitcells, atomic positions, andbonds, handling of multiple structural models using Vesta software.
5. HandsontrainingonX-pert High-scoresoftwareforXRDanalysis.

6. To search, analyze and curating chemical information, as well as for accessing spectraldata, synthetic methods, and safety information using ChemSpider, and Mendeley.

Reference(Theory):

1. Handbook for LaboratorySafety, Benjamin R. Sveinbjornsson and Sveinbjorn Gizurarson, Copyright © 2022 Elsevier Inc. ISBN 978-0-323-99320-3

2. LaboratorySafetyforChemistryStudents, RobertH.HillandDavidFinster,Wiley–Blackwell (20August 2010). ISBN-13:978-0470344286.
3. https://csl.du.ac.in/
4. https://www.youtube.com/watch?v=hhfckQtdfKw

References(Practical):

1. https://www.youtube.com/watch?v=fHEe7AZ7sS0
2. https://www.youtube.com/watch?v=8tCUg2B523o
3. https://share.google/NiP4QGBFQFT8wZnZm
4. https://www.youtube.com/watch?v=TwVyvh628wE
5. https://www.acdlabs.com/resources/free-chemistry-software-apps/chemsketch-freeware/(Freeware software)
6. https://www.youtube.com/watch?v=l06ljePcg8U
7. https://www.youtube.com/watch?v=CpW7khVmSAE
8. https://www.youtube.com/watch?v=dASaENblC_4
9. https://www.youtube.com/watch?app=desktop&v=TpuL4NgCMYc&t=0s
10. https://www.youtube.com/watch?v=lST-yMe322Y
11. https://www.youtube.com/watch?v=Go-BdmnYusU
12. https://www.youtube.com/c/mendeley/videos
13. https://www.youtube.com/watch?v=PJXnfBSq4Lg

*Students are encouraged to participate in various chemistry related workshops/conferences and submit their certificates and learning outcomes (1 page).

Assessmentmethods:Allexaminationandassessmentsmethodsshallbeinlinewiththe University of Delhi guidelines issued from time to time.

SKILLENHANCEMENTCOURSE(CH-SEC-108)

CREDITDISTRIBUTION,ELIGIBILITY,ANDPRE-REQUISITESOFTHECOURSE

Coursetitle&Code	Credits	Creditdistributionofthe course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
BestPracticesin Chemical LaboratorySafety **CH-SEC-108**	**2**	**1**	**0**	**1**	U.G. Chemistry	NIL

Course Objectives: For a majority of students, chemistry laboratory safety is limited to a set of safety precautions explained by the instructors during a chemistry practical class. These safety precautions, though important are not sufficient to prepare a student for a research laboratoryoranindustrialjobinthefieldofchemistry.Thiscourseaimstoprovideanin-depth knowledge on the best practices in chemistry laboratory safety. The students will be made awareoftheneedforsafetyculturethroughvariousdocumentedlaboratoryaccidentsandnear misses.Thiscoursewilldelveintorecognitionofhazards,riskassessmentanditsminimization in a chemistry laboratory through lectures, hands on learning/ demonstration and activities. This course will also prepare the students for responding to a chemical emergency.

LearningOutcomes:

After the completion of this course the students will develop a positive attitude towards safe laboratory practices. They will be able to recognise the potential hazards in a chemistry laboratory,assessthesehazardsbyGHS,SDSsandotherresourcesandwillbeabletominimise the risks. This course will also prepare them to respond to any emergencies in a chemistry laboratory. The students will also learn about chemical laboratory safety through hands on training, demonstration and activities. This advance course on best practices in chemistry laboratory safety will make students more employable in the field of chemistry in both academia and industry.

SYLLABUSOFCH-SEC-108

THEORYCOMPONENT **(1Credit:15Hours)**

UNIT1: **(15 Hours)**

LABORATORYSAFETYCULTURE

UnderstandingRAMPstrategy,ethicsandsafety,learningfromlabincidents.

RECOGNIZINGHAZARDS

GloballyHarmonizedSystemofClassificationandLabellingofChemicals(GHS)andSafety Data Sheets (SDSs); toxicity, corrosives, carcinogens, biological hazards, hazards of nanomaterials,flammablechemicals,incompatiblechemicals,explosionhazards,reactiveand unstable chemicals, gas cylinders, cryogenic liquid tanks, cryogenic hazards, low- or high-pressure systems.

ASSESSINGRISK

Understanding Occupational Exposure Limits (OEL), assessing chemical exposure, risk assessment for new experiments.

MINIMIZINGRISK

Strategies to minimise risk, Personal Protective Equipment (PPE), fume hood, common laboratorysafetymeasures in a chemistrylaboratory, handling chemical wastes, management of chemicals in a laboratory- chemical inventory, storage and chemical security.

PREPAREFOREMERGENCIES

Respondingto emergencies in a chemistrylaboratory, chemical spills, fire emergencies, first-aid.

PRACTICALCOMPONENT (1Credit:30 Hours)

1. Demonstration/handsonlearningofthe:

   a. Appropriate use of common laboratory devices and equipment (e.g., Bunsen burners, laboratoryovens,magneticstirrers,U.V.chambers,centrifuges,vacuumpumps,rotary evaporators, refrigerators, freezers etc.).
   b. Properuseof asafetyshower andan eyewash.
   c. Basicfirstaidproceduresforcommonminorlaboratoryaccidents
   d. Properdisposalof“sharps”andprevention oflacerationswhilehandlingglassware.
   e. Propertechniquesforcleaningupminorspills(acid,base,ororganicspill)inthe laboratory.
   f. AppropriateuseofPPEinresponsetoaminorchemicalspill.
   g. Properuseof thefireextinguisher.
   h. Storage protocols for laboratory chemicals (incompatible chemicals, flammables and corrosives)

2. UnderstandingRiskAssessment inalaboratorythrough activities.

3. SafetyData Sheet practicefora fewcommonlyused laboratorychemicals.

ESSENTIAL/RECOMMENDEDREADINGS

1. LaboratorySafetyforChemistryStudentsbyDavidFinsterandRobertHill. https://institute.acs.org/acs-center/lab-safety/education-training/college-univ-guidelines/laboratory-safety-for-chemistry-students-etextbook.html
2. Hill, R.H.; Finster, D.C.Laboratory Safety for Chemistry Students, 2nd Ed; Wiley:Hoboken, NJ, 2016.
3. Guidelines forChemical LaboratorySafetyinAcademic Institutions,ACS Committee on Chemical Safety, Washington, DC., 2016. www.acs.org/content/dam/acsorg/about/governance/committees/chemicalsafety/publications/acs-safety-guidelines-academic.pdf?logActivity=true
4. Safetyinacademicchemistrylaboratories8theditionbestpracticesforfirst-and second-year university student. https://www.acs.org/content/dam/acsorg/about/governance/committees/chemicalsafety/publications/safety-in-academic-chemistry-laboratories-students.pdf
5. Prudent practices in the laboratory: Handling and management of chemical hazards, Updated version. Washington, DC: The National Academies Press. https://doi.org/10.17226/12654.
6. United Nations. Globally Harmonized System of Classification and Labelling of Chemicals (GHS), Fifth revised edition, ST/SG/AC.10/30/Rev.5; New York and Geneva, 2013.
7. Bretherick's Handbook of Reactive Chemical Hazards, 8th Edition; Urben, P., Ed.; Elsevier, 2017.

Assessmentmethods: Allexaminationandassessmentsmethodsshallbeinlinewiththe University of Delhi guidelines issued from time to time.

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SKILLENHANCEMENTCOURSE(SEC)

CREDITDISTRIBUTION,ELIGIBILITY,ANDPRE-REQUISITESOFTHECOURSE

Coursetitle&Code	Credits	Creditdistributionofthecourse			Eligibility criteria	Pre-requisiteof the course (ifany)
		Lecture	Tutorial	Practical /Practice		
Introduction to Computer Programmingand Numerical Methods CH-SEC-109	**02**	**01**	**-**	**01**	U.G. Chemistry	10+2 in Science with Mathematics

Course Objectives

- To introduce the evolution of programming languages and the rationale behind structured programming.
- To familiarize students with the syntax, compilation/execution process, and development environments for programming, variables, data types, operators, expressions, and program structure
- Understand the fundamental principles and need fornumerical methods in solving mathematical problems.
- Developtheabilitytoimplementnumericalmethodsusingprogramming tools.

Learning Outcome

1) Write,compile,andexecutebasicprogramsusingappropriateIDEsandcompilers across different platforms.
2) Designmodularcodeusinguser-definedfunctions,input/outputoperations,control statements and formatted data handling
3) Explaintheconceptsandimportanceofnumericalmethodsincomputational problem-solving.
4) Applynumerical techniquesforsolving equations
5) Implementnumericalmethodsusingsuitableprogramminglanguagesortools.

Theory Component **Credit:1(15hours)**

Unit I:

A. Computer Programming: Evolution of programming languages; Importance of structured programming; Syntax overview and compilation/execution flow; IDEs and compilers. VariablesandDataTypes(constants;variables,anddeclarations);Integer,real,double, character,logical,Mix-modearithmeticandtypeconversion;Commentsandprogram structure; OperatorsandExpressions,Logical and arithmetic expressions, Built-in (library) functions;ControlStructures(Conditionalbranching,Loops),Input/OutputOperations,Concepts of Functions, Procedures, and Modular Programming;Arrays and Strings

B. Finding roots of an equation, Iterative method, Successive bisection method, Method offalse position and Newton-Raphson method.

RecommendedTexts/References:

1) Rajaraman,V.,*ComputerProgramminginC*.PHILearning;2nd edition(2019)
2) Kanetkar,Y.P.*LetusC*,BPBPublications;15thedition(2024)
3) Rajaraman,V.,*ComputerProgramminginFortran90and95*.2nd Edition,PHI Learning (1997)
4) Chapman,S.J.,*Fortran90/95forScientistsandEngineers*,McGraw-HillHigher Education; 2nd edition (2003)
5) Zelle, J. M. *Python Programming:An Introduction to Computer Science*, 4th Edition, Shroff Publishers & Distributors Pvt. Ltd. (2024)
6) Schatzman,M., *NumericalAnalysis:AMathematical Introduction*,1st edition, Oxford University Press. (2002).
7) Press,W.H.,Teukolsky,S.A.,Vetterling,W.T.andFlannery,B.P.,*NumericalRecipes: TheArtofScientificComputing*,Vol1,3rd Edition,CambridgeUniversityPress(2007).

LabComponents **Credit:1**

1) Write a program to compute (i) the area and circumference of a circle, given the radius,(ii)tocheckwhetheranumberispositive,negative,orzero,(iii) *H*and*S*from *Cp* from given data, (iv) *p*H of a weak and strong acid, (v) convert Celsius to Fahrenheit or vice versa, (vi) leap year checker, (vii) palindrome checker, (viii) Fibonacci series
2) Writeafunctiontocomputethefactorialofanumber.
3) Writeaprogramtoreverseagiven string.
4) Calculatethesumofthefirst10naturaland prime numbersusingaloop.
5) Writeaprogramtocheck whetheragivennumberisevenorodd.
6) Writeaprogramtofindthemaximumandminimaforasetof numbers.
7) Writeaprogramtofindarootusingthebisectionmethod.
8) Writeaprogramforfalsepositionmethodforroot-finding.
9) Writeaprogramtosolveanonlinearequationusingthefixed-pointiteration(simple iteration) method
10) UsetheNewton-Raphsonmethodtosolvesystemsofsimultaneousnonlinear equations.
11) ImplementandcomparetheBisectionandNewton-Raphsonmethodsforsolving nonlinear equations.
12) WriteaprogramtocompareBisection,RegulaFalsi,andNewton-Raphsonmethods on the same function.

RecommendedTexts/References:

1) Rajaraman,V.,*ComputerProgramminginC*.PHILearning;2nd edition(2019)
2) Kanetkar,Y.P.*LetusC*,BPBPublications;15thedition(2024)
3) Rajaraman,V.,*ComputerProgramminginFortran90and95*.2nd Edition,PHI Learning (1997)
4) Chapman,S.J.,*Fortran90/95forScientistsandEngineers*,McGraw-HillHigher Education; 2nd edition (2003)
5) Zelle, J. M. *Python Programming:An Introduction to Computer Science*, 4th Edition, Shroff Publishers & Distributors Pvt. Ltd. (2024)
6) Schatzman,M., *NumericalAnalysis:AMathematical Introduction*,1st edition, Oxford University Press. (2002).
7) Press,W.H.,Teukolsky,S.A.,Vetterling,W.T.andFlannery,B.P.,*NumericalRecipes: TheArtofScientificComputing*,Vol1,3rd Edition,CambridgeUniversityPress(2007).