

B.Sc. CHEMISTRY

CHOICE BASED CREDIT SYSTEM (CBCS)

Syllabus
2019-2020



DEPARTMENT OF CHEMISTRY
FACULTY OF ARTS, SCIENCE AND HUMANITIES

KARPAGAM ACADEMY OF HIGHER EDUCATION

(Deemed to be University)
(Established under section 3 of UGC Act, 1956)
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DEPARTMENT OF CHEMISTRY

FACULTY OF ARTS, SCIENCE AND HUMANITIES

UG PROGRAM (CBCS) – B.Sc. Chemistry (2019–2020 Batch and onwards)

Course code	Name of the course	Objectives & Outcomes		Instruction hours per week			Credits	Maximum Marks		
		PEO's	PO's	L	T	P			CI A	ES E
SEMESTER I										
19LSU101	Language –I	4	7	4	0	0	4	40	60	100
19ENU 101	English	4	7	4	0	0	4	40	60	100
19CHU101	Mathematics I	1,4	1,4,5,10	4	0	0	4	40	60	100
19CHU102	Inorganic Chemistry I:Atomic structure and Chemical Bonding	1	1,3	5	0	0	5	40	60	100
19CHU103	Organic Chemistry I: Basics and Hydrocarbons	1	1,3	5	0	0	5	40	60	100
19CHU111	Mathematics I Practical	2,3	2,5,9	0	0	4	2	40	60	100
19CHU112	Atomic structure and Chemical Bonding- Practical	1	1,4,10	0	0	2	1	40	60	100
19CHU113	Basics and Hydrocarbons-Practical	1	1,4,10	0	0	2	1	40	60	100
	Semester total						26	320	480	800
SEMESTER II										
19LSU201	Language –II			4	0	0	4	40	60	100
19CHU201	Mathematics II	1,4	1,4,5,10	4	0	0	4	40	60	100
19CHU202	Physical Chemistry II: Chemical Thermodynamics and its Application	1,2	2,5,10	5	0	0	5	40	60	100
19CHU203	Organic Chemistry II: Oxygen Containing Functional Groups	1,2	2,5	6	0	0	6	40	60	100
19CHU211	Mathematics II- Practical			0	0	4	2	40	60	100
19CHU212	Chemical Thermodynamics and its Application- Practical	1,2,3	2,3,4,9	0	0	2	1	40	60	100
19CHU213	Oxygen Containing Functional Groups- Practical	1,2,3	2,3,4,9	0	0	2	1	40	60	100
19AEC201	Environmental Studies	2	-	3	0	0	3	40	60	100
	Semester Total						26	320	480	800
SEMESTER III										
19CHU301	Physics- I	1,2,3	2,3,4,10	04	0	0	4	40	60	100
19CHU302	Inorganic Chemistry III: Coordination Chemistry	1,2,3	2,3,4,10	04	0	0	4	40	60	100
19CHU303	Physical Chemistry III: Phase Equilibria and Chemical Kinetics	1,2,3	2,3,4,10	04	0	0	4	40	60	100
19CHU311	Physics- I Practical	1,2,5	2,3,4,9	0	0	4	2	40	60	100
19CHU312	Coordination Chemistry- Practical	1,2	2,3,4,9	0	0	4	2	40	60	100
19CHU313	Phase Equilibria and Chemical Kinetics- Practical	1,2	2,3,4,9	0	0	4	2	40	60	100
19CHU304A	Pharmaceutical chemistry	1,2,3	2,3,6,	03	0	0	3	40	60	100

19CHU304B	IT skills for chemists		10							
19CHU314A	Pharmaceutical chemistry- Practical	1,2,3	2,3,6, 10	0	0	3	1	40	60	100
19CHU314B	IT skills for chemists- Practical									
	Semester total						22	320	580	900
SEMESTER IV										
19CHU401	Physics II	2,3	2,3,4	04	0	0	4	40	60	100
19CHU402	Physical Chemistry IV: Electrochemistry	1,2,3	1,2,4, 5,9	04	0	0	4	40	60	100
19CHU403	Organic Chemistry IV : Organic Spectroscopy	1,2,3	2,3,4, 6	04	0	0	4	40	60	100
19CHU411	Physics II- Practical	2,5	2,3,4	0	0	4	2	40	60	100
19CHU412	Physical Chemistry IV: Electrochemistry- Practical	1,2,3	2,3,4, 5,6	0	0	4	2	40	60	100
19CHU413	Organic Spectroscopy- Practical	1,2,3	2,4,6, 7,8	0	0	4	2	40	60	100
19CHU404A	Green Methods in Chemistry	1,2,3	1,3,6, 8,9	03	0	0	3	40	60	100
19CHU404B	Analytical clinical Biochemistry	1,2,3	1,2,3, 10							
19CHU414A	Green Methods in Chemistry- Practical	1,2,3	1,3,6, 8,9	0	0	3	1	40	60	100
19CHU414B	Analytical clinical Biochemistry- Practical	1,2,3	1,2,3							
	Semester total						22	320	480	800
SEMESTER V										
19CHU501A	Cheminformatics	1,2,3	1,2,5, 8,10	03	0	0	3	40	60	100
19CHU501B	Chemistry of Cosmetics and perfumes	1,2,3,	2,3,7							
19CHU511A	Cheminformatics- Practical	2,3	1,2,5, 8	0	0	3	1	40	60	100
19CHU511B	Chemistry of Cosmetics and perfumes- Practical	2,3	2,3,7, 9							
19CHU502A	Polymer Chemistry	1,2,3	2,3,4, 7,8	04	0	0	4	40	60	100
19CHU502B	Novel inorganic Solids	1,2,3	3,4,7							
19CHU503	Nitrogen containing functional groups, Heterocyclic Chemistry and Natural products	1,2,3	2,3,4, 5,6	04	0	0	4	40	60	100
19CHU504	Inorganic Chemistry II:Metallurgy, s-block and p-block Elements	1,2,3	2,3,5, 7,8	04	0	0	4	40	60	100
19CHU512A	Polymer Chemistry- Practical	1,2,3	2,3,4, 5,6	0	0	4	2	40	60	100
19CHU512B	Novel inorganic Solids- Practical	2,3	3,4,7, 9							
19CHU513	Nitrogen containing functional groups, Heterocyclic Chemistry and Natural products – Practical	1,2,3	2,3,9	0	0	04	2	40	60	100

19CHU514	Inorganic Chemistry II: Metallurgy, s-block and p-block Elements - Practical			0	0	04	2	40	60	100
	Semester Total						22	320	480	800
SEMESTER VI										
19CHU601A	Basic Analytical Chemistry	1,2,3	2,4,5	03	0	0	3	40	60	100
19CHU601B	Pesticide Chemistry	1,2,3	3,6,7							
19CHU611A	Basic Analytical Chemistry- Practical	1,2,3	2,4,5	0	0	3	1	40	60	100
19CHU611B	Pesticide Chemistry- Practical	1,2,3	3,6,7							
19CHU602	Inorganic Chemistry IV: Organometallic Chemistry	1,2,3	2,3,4, 5,6	04	0	0	4	40	60	100
19CHU603	Physical Chemistry I: States of Matter and Ionic Equilibrium	1,2,3	2,3,4, 5,7	04	0	0	4	40	60	100
19CHU612	Organometallic Chemistry- Practical	1,2	2,3,4, 9	0	0	04	2	40	60	100
19CHU613	Physical Chemistry I: States of Matter and Ionic Equilibrium- Practical	1,2	2,3,4, 9	0	0	04	2	40	60	100
19CHU604	Molecular modeling and drug design	1,2,3	1,3,6, 8	0	0	8	6	40	60	100
19CHU614	Molecular modeling and drug design practical	1,2,3	2,3,6							
19CHU691	Project work	1,2,3, 4	1,2,3, 5,6,8							
							22	280	420	700
ECA / NCC / NSS / Sports / General interest etc										Good
	G. Total						140	1880	2820	4700

Skill Enhancement Elective Courses			
Elective	Semester	Course Code	Name of the Course
SEC-1	III	19CHU304A	Pharmaceutical chemistry
		19CHU304B	IT skills for chemists
	III	19CHU314A	Pharmaceutical chemistry Practical
		19CHU314B	IT skills for chemists Practical
SEC- 2	IV	19CHU404A	Green Methods in Chemistry
		19CHU404B	Analytical clinical Biochemistry
	IV	19CHU414A	Green Methods in Chemistry practical
		19CHU414B	Analytical clinical Biochemistry Practical
SEC-3	V	19CHU501A	Cheminformatics
		19CHU501B	Chemistry of Cosmetics and perfumes
	V	19CHU511A	Cheminformatics practical
		19CHU511B	Chemistry of Cosmetics and perfumes Practical
SEC-4	VI	19CHU601A	Basic Analytical Chemistry
		19CHU601B	Pesticide Chemistry

	VI	19CHU611A	Basic Analytical Chemistry Practical
		19CHU611B	Pesticide Chemistry Practical
Generic Elective/Allied Courses			
Elective	Semester	Course Code	Name of the Course
GEC-1	I	19CHU101	Mathematics I
		19CHU111	Mathematics I Practical
GEC-2	II	19CHU201	Mathematics II
		19CHU211	Mathematics II practical
GEC-3	III	19CHU301	Physics I
		19CHU311	Physics I Practical
GEC-4	IV	19CHU401	Physics II
		19CHU411	Physics II Practical

CORE COURSE

- CC-1 : Inorganic Chemistry I: Atomic structure and Chemical Bonding
 CC-2 : Organic Chemistry I: Basics and Hydrocarbons
 CC-3 : Physical Chemistry II: Chemical Thermodynamics and its Application
 CC-4 : Organic Chemistry practical II: Oxygen Containing Functional Groups
 CC-5 : Inorganic Chemistry III: Coordination Chemistry
 CC-6 : Physical Chemistry III: Phase Equilibria and Chemical Kinetics
 CC-7 : Physical Chemistry IV: Electrochemistry
 CC-8 : Organic Chemistry: Organic Spectroscopy
 CC-9 : Organic Chemistry III : Heterocyclic Chemistry
 CC-10 : Inorganic Chemistry Practical II Inorganic Chemistry II: s-block and p-block Elements
 CC-11 : Inorganic Chemistry IV: Organometallic Chemistry
 CC-12 : Physical Chemistry I: States of Matter and Ionic Equilibrium

SKILL ENHANCEMENT COURSE

- SEC-1 : Pharmaceutical chemistry
 SEC-2 : IT skills for chemists
 SEC-3 : Green Methods in Chemistry
 SEC-4 : Analytical clinical Biochemistry
 SEC-5 : Cheminformatics
 SEC-6 : Chemistry of Cosmetics and perfumes
 SEC-7 : Basic Analytical Chemistry
 SEC-8 : Pesticide Chemistry

GENERIC ELECTIVE /ALLIED COURSES

- GEC-1 : Mathematics I
 GEC-II : Mathematics II
 GEC III: Physics I

DISCIPLINE SPECIFIC ELECTIVE

DSE-1 : Polymer Chemistry

DSE-2 : Novel inorganic Solids

DSE-3 : Molecular modelling and drug design

DSE-4 : Project

Programme Outcome

1. Have firm foundations in the fundamentals and application of current chemical and scientific theories.
2. Are able to design, carry out, record and analyze the results of chemical experiments.
3. Knows the proper procedures and regulations for safe handling and use of chemicals and can follow the proper procedures and regulations for safe handling when using chemicals.
4. Students should have a working knowledge of the main areas of chemistry: organic, inorganic, analytical, and physical.
5. Students should possess critical thinking and problem solving abilities.
6. Students should be able to perform and understand chemical research.
7. Students should be able to describe, both in writing and orally, chemical processes and procedures
8. Students should be able to work in a chemical or related field.

Programme specific Outcome

9. Are able to use modern instrumentation and classical techniques, to design experiments, and to properly record the results of their experiment.
10. Students should have a basic level understanding of the following areas of chemistry - Analytical, Inorganic, Organic, and Physical Chemistry.
11. Students should be able to work in a chemical or related field.

Programme Educational Objectives

PEO-1

Acquire the fundamental principles of science and demonstrate broad knowledge of descriptive chemistry and will be able to nurture the needs of industries/laboratories related to chemistry

PEO-2

To motivate critical thinking and analytical skills to solve chemical problems of practical relevance to society while complying with economical, environmental, ethical, and safety factors.

PEO-3

To synthesize, separate and characterize compounds using published reactions, protocols, standard laboratory equipment, and modern instrumentation.

PEO-4

Demonstrate professional excellence, ethics and will be able to communicate effectively the scientific information and research results in written and oral formats, to both professional scientists and to the public.

Mapping

PO's	a	b	c	d	e	f	g	h	i	j	k
PEO 1	X	X	X	X			X		X	X	
PEO 2					X		X		X		
PEO 3		X				X			X		X
PEO 4						X	X	X		X	X

Blue- Employability

Green- Entrepreneurship

Red – Skill development

பகுதி - I, தமிழ்ப்பருவம் I

19LSU101 :

தமிழ்முதல்தாள்

4-H,4-C

(இளநிலை அறிவியல் பட்ட வகுப்புகளுக்குரியது)

பாடத்திட்டப் பொதுநோக்கம்

- கற்றல் வழி சிந்தனைத் திறனையும், கருத்து வெளிப்பாட்டுத் திறனையும், மேம்படுத்துதல்.
- ஆய்வுநோக்கை மேம்படுத்துதல்.
- இலக்கியங்கள் உணர்த்தும் வாழ்வின் நுட்பமான பகுதிகளை உணர்த்துதல்.
- மனித மனத்தினைப் பக்குவப்படுத்துதலில் இலக்கியம் தரும் பங்கினை உணர்த்துதல்.
- வளர்ந்து வரும் சமூகத்தில் அறஉணர்வு, பண்பாடு போன்றவை குறித்து அறிவூட்டல்.
- அரசுத் தேர்வுகளுக்கு மாணவர்களை ஆயத்தமாக்குதல்.

பாடத்திட்டப் பயன் விளைவு

1. இந்திய குடியுரிமைப் பணி முதலான போட்டித் தேர்வுகளில், விருப்பப் பாடமாக இடம்பெறுகின்ற, 'தமிழ் இலக்கிய வரலாறு' குறித்த முழுமையான அறிமுகம் பெற்றிருத்தல்.
2. கல்வெட்டியல், ஓலைச்சுவடியியல் மற்றும் தொல்லியல் சார்ந்த ஆவணத் தேடலுக்குரிய ஆய்வுமனப்பான்மையுடன், இலக்கியங்களை அணுகுதல்.
3. தமிழின் வளர்ச்சித் துறையாகிய, 'அறிவியல் தமிழ்' ; 'இணைய தமிழ்' குறித்த பன்னோக்கு அணுகுமுறையிலான ஆய்வுச் சிந்தனை மேம்பாடு.
4. வேலைவாய்ப்புக்குரிய சுயதிறன் மேம்பாட்டுடன், படைப்பாக்கத்திறன் மேம்பாடும் பெற்றிருத்தல் .
5. சமுதாய மற்றும் வாழ்வியல் மதிப்புகளைப் பேணுவதற்குக் கருவியாக இலக்கியங்களை நாடுகின்ற மனப்பான்மை வளர்ச்சி.
6. மொழிபெயப்புத் துறைசார்ந்த வேலைவாய்ப்புத் திறன் பெற்றிருத்தல்

அலகு - I :இக்காலஇலக்கியம்:

(10 மணிநேரம்)

கல்வி	:	மகாகவிபாரதியார் - சுயசரிதை -ஆங்கிலக் கல்வி.
இன்றைய நிலை	:	கவிமணி தேசிக விநாயகம் பிள்ளை-ஒற்றுமையே உயிர்நிலை.
மனிதநேயம்	:	கவிஞர்சிற்றிபாலசுப்பிரமணியன் -மலையாளக் காற்று.
சூழலியல்	:	கவிஞர்வைதீஸ்வரன் - விரல் மீட்டிய மழை.
பெண்ணியம்	:	கவிஞர்சுகந்தி சுப்பிரமணியம் - புதையுண்ட வாழ்க்கை.

அலகு - II :அறஇலக்கியம்:

(10 மணிநேரம்)

கொன்றை வேந்தன்: 1-50 பாடல்கள்

திருக்குறள்: பண்புடைமை, வினைத்திட்டம் - 20 குறள்கள்

பழமொழி நானூறு: 5 பாடல்கள்

அலகு - III :சிற்றிலக்கியம்:

(10 மணிநேரம்)

மூவருலா: 1-26 கண்ணிகள்

திருச்செந்தூர் முருகன் பிள்ளைத்தமிழ்: 2 பாடல்கள்

கலிங்கத்துப் பரணி: போர்பாடியது - 9 பாடல்கள்

அலகு - IV :கட்டுரை:

(10 மணிநேரம்)

1. உயர்தனிச் செம்மொழி - பரிதிமாற்கலைஞர்
2. கட்டிடக்கலை - அ. இராசமாணிக்கனார்
3. வாழ்க்கை - இளவழகனார்
4. ஆளுமைத்திறன் அறிவோம் - ஸ்ரீகண்ணன்
5. மணற்கேணி - நெ.து.சுந்தரவடிவேலு

அலகு- V :மொழிப்பயிற்சி:

(8 மணிநேரம்)

1. படைப்பிலக்கியப் பயிற்சிகள் (கதை,கவிதை, கட்டுரை, உரைநடை)
2. மொழிபெயர்ப்பு
3. இலக்கணப் பயிற்சிகள்

பாடநூல்:கற்பகச்சோலை – தமிழ்ஏடு.கற்பகம்பல்கலைக்கழகத்தமிழ்த்துறைவெளியீடு.

19ENU101	Semester-I ENGLISH	4H – 4C
Instruction Hours / week: L: 4 T: 0 P: 0	Marks: Internal: 40	External: 60 Total: 100
End Semester Exam: 3 Hours		

Course Objectives

- To enable the learners to acquire English language skills at a faster pace.
- To train the learners to reflect on the literary works and communicate flexibly.
- Know about the Prose and Poetry
- To develop the Short Story:
- Learn about Vocabulary, Grammar and Composition:
- Know about Proverb Expansion

Course Outcomes

1. Enable the learners to acquire English language skills at a faster pace.
2. Trained the learners to reflect on the literary works and communicate flexibly.
3. Knowledge about the Prose and Poetry
4. Development of the Short Story:
5. Learnt about Vocabulary, Grammar and Composition:
6. Knowledge about Proverb Expansion

UNIT - I : PROSE

1. Morals in the Indian Context - Francis Nicholas Chelliah
2. How Comic Books help us to relive our Childhood - Benoit Peeters
3. Let's Do What India Needs From Us -Dr.A.P.J. Abdul Kalam

UNIT - II : POEM

1. The Stolen Boat - William Wordsworth
2. Telephone Conversation- Wole Soyinka
3. A River - A.K. Ramanujan

UNIT - III : SHORT STORIES

1. Rapunzel - Brothers Grimm
2. The Ant and The Grasshopper- W. Somerset Maugham
3. The Nightingale and the Rose - Oscar Wilde.

UNIT - IV: Drama

1. The Merchant of Venice- Act 4-Scene 1
2. The Death Trap- Saki

UNIT - V: Grammar and Composition

- GRAMMAR : 1. Tenses
2. Articles
 3. Auxiliaries (Primary and Modal)
 4. Tag Questions

Composition:

1. Reading to Comprehend
2. Letter Writing
3. Resume Writing
4. General Essay

Prescribed Text: Reminisce, Published by the Department of English, Karpagam Academy of Higher Education.

Suggested Reading: Hewings Martin, 1999 Advanced English Grammar, Cambridge University Press

19CHU101	MATHEMATICS I:	Semester-I 4H 4C
<hr/>		
Instruction Hours/week:L: 4 T:0 P:0	Marks: Internal:40 External: 60	Total:100
End Semester Exam: 3 hrs		

Course Objectives

Students should be able

- Mathematics is an important tool for the study of physics and Chemistry.
- Basic mathematical tools like vector analysis
- Matrices
- Complex variables and analysis etc.
- Differential Calculus
- Integral Calculus

Course Objective:

To give a strong basic foundation in mathematics which is very much necessary to study any subject in Physics.

1. Important tool for the study of physics and Chemistry.
2. Basic mathematical tools like vector analysis
3. Matrices
4. Complex variables and analysis etc.
5. Differential Calculus
6. Integral Calculus

UNIT I

Matrices: Different types of matrices – Inverse of a matrix – Solution of simultaneous equations by matrix method- Cayley-Hamilton theorem(Statement only)-Verification.

UNIT II

Vector calculus: Concepts of vector and scalar fields- Derivative of a vector - The Del operator, Gradient – Divergence of a vector – Curl of a vector- Directional derivative – Formula involving ∇ operator. Laplacian Operator.

UNIT III

Complex variables: Analytical function –Cauchy –Reimann equations – The necessary and sufficient condition for $f(z)$ to be analytic – Polar form of C-R equation-Properties of analytic function – Construction of analytic functions – Milne Thomson method.

UNIT IV

Differential calculus: Differentiation- Curvature and radius of Curvature in Cartesian and Polar form – Evolutes – Involute.

UNIT V

Integral Calculus: Definite and Indefinite integrals – Methods of Integration – Integration by substitution – Integration by parts.

Text Books

1. Venkataraman. M. K.,1998. Engineering Mathematics, The National Publications & Co., Chennai. (Unit I, II)
2. Manickavasagam Pillai.T.K , and S. Narayanan, 2002.“Calculus”, Volume I, and Volume II S.V Printers & Publishers, Chennai (Unit IV, V)
3. Sastry .S.S, 2009, Engineering mathematics, PHI learning Pvt. Ltd, New Delhi (Unit III)

Semester-I

19CHU102INORGANIC CHEMISTRY I: Atomic structure and chemical bonding 5H 5C**Instruction Hours/week:L:5 T:0 P:0Marks: Internal:40 External: 60 Total:100****End Semester Exam: 3 hrs****Course Objectives**

Students should be able

- To discuss the limitations of classical mechanics and its drawbacks.
- To discuss the radial and angular part of orbitals
- To explain the fundamentals of quantum mechanics and Schrödinger equation for simple atoms.
- To predict and write the electronic configuration of elements.
- To explain a different types of bonding like ionic and covalent bonding.
- To interpret a knowledge about the various theories of bonding like VSEPR, Valence Bond Theory and Molecular Orbital Theory of covalent bonding.

Course Outcomes

1. Explain the atomic theory of matter, composition of the atom, which defines the identity of a given element.
2. Understood the radial and angular part of orbitals
3. Explain the relative sizes, masses, and charges of the proton, neutron, and electron, and their assembly to form different atoms.
4. Define the term isotope, and their atomic and mass numbers.
5. Use the Periodic Table to rationalize similarities and differences of elements, including physical and chemical properties and reactivity.
6. Predict common ionic charges of group 1A, 2A, 3A, 6A, and 7A elements based on position in the periodic table.

Atomic Structure:**UNIT I**

Review of: Bohr's theory and its limitations, dual behaviour of matter and radiation, de Broglie's relation, Heisenberg Uncertainty principle. Hydrogen atom spectra. Need of a new approach to atomic structure. What is Quantum mechanics? Time independent Schrodinger equation and meaning of various terms in it. Significance of ψ and ψ^2 , Schrödinger equation for hydrogen atom. Radial and angular parts of the hydrogenic wavefunctions (atomic orbitals) and their variations for $1s$, $2s$, $2p$, $3s$, $3p$ and $3d$ orbitals (Only graphical representation). Radial and angular nodes and their significance. Radial distribution functions and the concept of the most probable distance with special reference to $1s$ and $2s$ atomic orbitals.

UNIT II

Significance of quantum numbers, orbital angular momentum and quantum numbers ml and ms . Shapes of s , p and d atomic orbitals, nodal planes. Discovery of spin, spin quantum number (s) and magnetic spin quantum number (ms). Rules for filling electrons in various orbitals, Electronic configurations of the atoms. Stability of half-filled and completely filled orbitals, concept of exchange energy. Relative energies of atomic orbitals, Anomalous electronic configurations.

Chemical Bonding and Molecular Structure

UNIT III

Ionic Bonding: General characteristics of ionic bonding. Energy considerations in ionic bonding, lattice energy and solvation energy and their importance in the context of stability and solubility of ionic compounds. Statement of Born-Landé equation for calculation of lattice energy, Born-Haber cycle and its applications, polarizing power and polarizability. Fajan's rules, ionic character in covalent compounds, bond moment, dipole moment and percentage ionic character

UNIT IV

Covalent bonding: VB Approach: Shapes of some inorganic molecules and ions on the basis of VSEPR and hybridization with suitable examples of linear, trigonal planar, square planar, tetrahedral, trigonal bipyramidal and octahedral arrangements. Concept of resonance and resonating structures in various inorganic and organic compounds.

UNIT V

MO Approach: Rules for the LCAO method, bonding and antibonding MOs and their characteristics for $s-s$, $s-p$ and $p-p$ combinations of atomic orbitals, nonbonding combination of orbitals, MO treatment of homonuclear diatomic molecules of 1st and 2nd periods (including idea of $s-p$ mixing) and heteronuclear diatomic molecules such as CO, NO and NO^+ . Comparison of VB and MO approaches.

Suggested Readings:

1. Lee, J.D. (2010). Concise Inorganic Chemistry. ELBS.
2. Cotton, F.A., Wilkinson, G. & Gaus, P.L. (2008). Basic Inorganic Chemistry. 3rd ed. John Wiley & sons.
3. Madan, R. L. (2015). Chemistry for Degree Students, S. Chand & Company Pvt. Ltd. Ram Nagar, New Delhi.
4. Douglas, B.E., McDaniel, D.H. & Alexander, J.J. (2010). Concepts and Models in Inorganic Chemistry. John Wiley & Sons.
5. Huheey, J.E., Keiter, E.A., Keiter, R.L. & Medhi, O.K. (2006). Inorganic Chemistry: Principles of Structure and Reactivity. Pearson Education India.

		Semester-I
19CHU103	ORGANIC CHEMISTRY I: Basics and Hydrocarbons	5H 5C
Instruction Hours/week: L:4 T:0 P:0 Marks: Internal:40 External: 60 Total:100		
End Semester Exam: 3 hrs		

Course objectives

- To describe knowledge on the basics of organic chemistry
- To gain knowledge in particularly the shapes of molecules, electron displacement effects, reagents, intermediates and fundamental types of reactions.
- To explain the students about the stereochemistry, projection formulae of molecules, geometrical isomerism and optical isomerism
- To explain the preparation and conformation analysis of alkanes.
- To paraphrase a knowledge about the preparation and properties of alkenes and alkynes, mechanisms of reactions and rules behind the reactions.
- To summarise a knowledge about the aromaticity of molecules and about electrophilic aromatic substitutions.

Course outcomes

1. Describe molecular structure and bonding in organic molecules.
2. Classify organic compounds by structure, use the IUPAC nomenclature, and identify conformational effects in organic compounds.
3. Predict the products of reactions of alkenes and describe the mechanisms showing how the products are formed.
4. Draw and interpret reaction coordinate diagrams, and relate the energetic changes associated with chemical reactions to equilibrium constants and rate; and differentiate kinetic versus thermodynamic control of reactions.
5. Identify the types of isomerism in organic compounds, to identify and classify chiral centers, and explain the physical and chemical consequences of chirality.
6. Correctly represent the structures and bonding of alkynes, and describe the mechanisms for reactions of alkynes and predict the products of such reactions.
7. Identify compounds in which resonance is important, predict the effect of resonance on the stability of compounds and reactive intermediates, and draw resonance structures.
8. Identify conjugated pi systems and explain the effect of conjugation on molecular structure and reactivity; and predict the products of reactions of dienes.
9. Describe mechanisms for substitution and elimination reactions, and predict the effect of nucleophile, leaving group, and solvent on the relative rates of S₁ versus S₂ reactions, and E₁ versus E₂ reactions, as well as on the relative rates of substitution versus elimination.

UNIT I**Basics of Organic Chemistry**

Hybridization, Shapes of molecules

Electronic Displacements: Inductive, electromeric, resonance and mesomeric effects, hyperconjugation and dipole moment; Hydrogen bonding (Applications to be discussed with relevant topics) Homolytic and Heterolytic fission with suitable examples. Curly arrow rules, formal charges; Electrophiles and Nucleophiles; Types, shape and relative stability of Carbocations, Carbanions, Free radicals and Carbenes. Introduction to types of organic reactions: Addition, Elimination and Substitution reactions.

UNIT II

Stereochemistry:

Fischer, Newmann and Sawhorse Projection formulae and their interconversions; Geometrical isomerism: cis-trans, syn-anti and E/Z notations with C.I.P rules.

Optical Isomerism: Optical Activity, Specific Rotation, Chirality/Asymmetry, Enantiomers, Molecules with two or more chiral-centres, Diastereoisomers, meso structures, Racemic mixture and their resolution. Relative and absolute configuration: D/L and R/S designations.

UNIT III

Chemistry of Aliphatic Hydrocarbons

Carbon-Carbon sigma bonds

General methods of preparation, physical and chemical properties of alkanes: Wurtz Reaction, Wurtz-Fittig Reactions, Free radical substitutions: Halogenation-relative reactivity and selectivity.

Cycloalkanes and Conformational Analysis

Conformational analysis of alkanes: Relative stability and Energy diagrams. Types of cycloalkanes and their relative stability, Baeyer strain theory: Chair, Boat and Twist boat forms of cyclohexane with energy diagrams; Relative stability of mono substituted cycloalkanes.

Unit IV

Chemistry of Aliphatic Hydrocarbons

Carbon-Carbon pi bonds:

General methods of preparation, physical and chemical properties of alkenes and alkynes, Mechanism of E1, E2, E1cb reactions. Saytzeff and Hofmann eliminations. Electrophilic additions and their mechanisms (Markownikoff/ Anti Markownikoff addition), mechanism of oxymercuration-demercuration, hydroboration-oxidation, ozonolysis, reduction (catalytic and chemical), syn and anti-hydroxylation (oxidation). 1,2- and 1,4-addition reactions in conjugated dienes and Diels-Alder reaction; Allylic and benzylic bromination and mechanism, e.g. propene, 1-butene, toluene, ethyl benzene.

Reactions of alkynes: Acidity, Electrophilic and Nucleophilic additions. Hydration to form carbonyl compounds, Alkylation of terminal alkynes.

UNIT V

Aromatic Hydrocarbons

Aromaticity: Hückel's rule, aromatic character of arenes, cyclic carbocations/carbanions and heterocyclic compounds with suitable examples. Electrophilic aromatic substitution: halogenation, nitration, sulphonation and Friedel-Craft's alkylation/acylation with their mechanism. Directing effects of the groups.

Suggested Readings:

1. Morrison, R. N. & Boyd, R. N. (2012). Organic Chemistry. India: Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Finar, I. L. (2012). Organic Chemistry. Volume 1. India: Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Madan, R. L. (2015). Chemistry for Degree Students, S. Chand & Company Pvt. Ltd. Ram Nagar, New Delhi.

4. Finar, I. L. (2012). Organic Chemistry: Stereochemistry and the Chemistry of Natural Products. Volume 2. India: Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
5. Eliel, E. L. & Wilen, S. H. (2010). Stereochemistry of Organic Compounds, Wiley. London
6. Kalsi, P. S. (2012). Stereochemistry Conformation and Mechanism. New Age International.
7. Jain M.K. & Sharma S.C. (2015). Modern Organic Chemistry, 4th Edition, Vishal publishing Co New Delhi.

19CHU111	MATHEMATICS I:PRACTICAL	Semester-I 4H 4C
<hr/>		
Instruction Hours/week:L: 0 T:0 P:4 Marks: Internal:40 External: 60 Total:100		
End Semester Exam: 3 hrs		

Course Objectives

This course enables the students

- To develop skills for quantitative estimation using computer language.
- To code various differentiation equation
- To code various intergration equation
- To code various differentiation and integration methods in a modern computer language.
- To plot the graphs of function
- To carryout the mean , median , standard deviations.

Course Outcomes (COs)

On successful completion of this course, the student will be able to

1. Solve complicated matrix related problems like matrix inverse and matrix multiplication.
Acquire problem-solving skills through computer programming.
2. Plot various functions and parametric curves.
3. Worked the various differentiation equation
4. Worked t the various integration equation
5. Woked the mean , median , standard deviations.

LIST OF PRACTICALS

1. Matrix addition.
2. Matrix subtraction.
3. Matrix multiplication.
4. Inverse of a matrix.
5. Mean
6. Median
7. Mode
8. Standard deviation.

19CHU112	ATOMIC STRUCTURE AND CHEMICAL BONDING - PRACTICAL	Semester-I
		2H 1C

Instruction Hours/week:L: 0 T:0 P:2Marks: Internal:40 External: 60 Total:100

End Semester Exam: 3 hrs

Course objectives

- To illustrate the principles of volumetric analysis.
- To categorize a versatile knowledge of solution preparations
- To prepare solutions with appropriate concentrations, titrations
- How to handle the apparatus while doing a titration.
- To analyse the knowledge about the calculations involved in the estimation of compounds using volumetric analysis.
- To estimate the amount of solution present quantitatively.

Course outcomes (CO's)

The Students are able

1. Summarize the principles of volumetric analysis.
2. Gained knowledge about the preparations of solutions
3. Understood the preparation of appropriate concentrations, titrations
4. Handled the respective apparatus while doing a titration.
5. Analyse the calculations involved in volumetric analysis and in the estimation of compounds using volumetric analysis.
6. The lab will also provide hands-on opportunities to develop and apply this knowledge

Inorganic Chemistry - Volumetric Analysis

1. Estimation of sodium carbonate and sodium hydrogen carbonate present in a mixture.
2. Estimation of oxalic acid by titrating it with KMnO_4 .
3. Estimation of water of crystallization in Mohr's salt by titrating with KMnO_4 .
4. Estimation of Fe (II) ions by titrating it with $\text{K}_2\text{Cr}_2\text{O}_7$ using internal indicator.
5. Estimation of Cu (II) ions iodometrically using $\text{Na}_2\text{S}_2\text{O}_3$.

Suggested Readings:

1. Svehla, G. (2012). Vogel's Qualitative Inorganic Analysis. Pearson Education.
2. Mendham, J. (2009) Vogel's Quantitative Chemical Analysis, Pearson.

19CHU113 BASICS AND HYDROCARBONS – PRACTICAL 2H 1C**Instruction Hours/week: L: 0 T: 0 P: 2 Marks: Internal: 40 External: 60 Total: 100****End Semester Exam: 3 hrs****Course objectives**

To develop skills in

- To perform the purification of organic compounds by crystallisation.
- To solve the calibration of the thermometer, determine the melting point, and to analyse the effect of impurities on the melting point.
- To predict the boiling point of a liquid by distillation method.
- To explain the principles of chromatography and to separate organic compounds by paper and thin layer chromatography.
- To detect the elements present in an organic compound.
- To demonstrate the preparation of few organic compounds using standard organic reactions.

Course Outcomes (CO's)

The student will be able to

1. Purify organic compounds by crystallisation.
 2. Characterisation of the compounds by elemental analysis, melting point, and effect of impurities on the melting point.
 3. Separation of organic compounds by paper chromatographic and TLC methods
 4. Preparation of organic compounds by standard organic reactions.
 5. The lab will also provide hands-on opportunities to develop and apply this knowledge.
 6. Understood the principles of chromatography and to separate organic compounds by paper and thin layer chromatography
-
1. Checking the calibration of the thermometer
 2. Purification of organic compounds by crystallization using the following solvents:
a. Water, b. Alcohol, c. Alcohol-Water
 3. Determination of the melting points of unknown organic compounds.
 4. Effect of impurities on the melting point – mixed melting point of two unknown organic Compounds
 5. Determination of boiling point of liquid compounds. (boiling point lower than and more than 100 °C by distillation)
 6. Chromatography
 - a. Separation of a mixture of two amino acids by ascending paper chromatography
 - b. Separation of a mixture of two sugars by ascending paper chromatography
 - c. Separation of a mixture of o- and p-nitrophenol or o- and p-aminophenol by thin layer chromatography (TLC)

7. Detection of extra elements
8. Organic Preparations
 - (i) Preparation of Benzophenoneoxime.
 - (ii) Preparation of Phenylbenzoate

Suggested Readings:

1. Mann, F.G. & Saunders, B.C.(2009). Practical Organic Chemistry.Pearson Education.
2. Veeraiyan V, Venkateswaran R, and Vaithiyalingam A.R. (2015). Basic Principles of Practical Chemistry, S. Chand & Sons Ltd.
3. Raj K. Bansal, (2012). Laboratory Manual of Organic Chemistry, New Age International Publishers (P) Ltd.
4. Thomas A.O. (2003). Practical Chemistry for B.Sc Main Students, Scientific Book Centre, Cannore-1, Kerala.
5. Furniss, B.S., Hannaford, A.J., Smith, P.W.G. & Tatchell A.R. (2012). Practical Organic Chemistry.5th Ed. Pearson.

பகுதி – I, தமிழ்ப்பருவம் || 19LSU201 : தமிழ் இரண்டாம் தாள் 4-H,4-C
(இளநிலை அறிவியல் பட்ட வகுப்புகளுக்குரியது)

பாடத்திட்டப் பொதுநோக்கம்

- கற்றல் வழி சிந்தனைத் திறனையும், கருத்து வெளிப்பாட்டுத் திறனையும், மேம்படுத்துதல்.
- ஆய்வுநோக்கை மேம்படுத்துதல்.
- இலக்கியங்கள் உணர்த்தும் வாழ்வின் நுட்பமான பகுதிகளை உணர்த்துதல்.
- மனித மனத்தினைப் பக்குவப்படுத்துதலில் இலக்கியம் தரும் பங்கினை உணர்த்துதல்.
- வளர்ந்து வரும் சமூகத்தில் அறஉணர்வு, பண்பாடு போன்றவை குறித்து அறிவூட்டல்.
- அரசுத் தேர்வுகளுக்கு மாணவர்களை ஆயத்தமாக்குதல்.

பாடத்திட்டப் பயன் விளைவு

1. இந்திய குடியுரிமைப் பணி முதலான போட்டித் தேர்வுகளில், விருப்பப் பாடமாக இடம்பெறுகின்ற, 'தமிழ் இலக்கிய வரலாறு' குறித்த முழுமையான அறிமுகம் பெற்றிருத்தல்.
2. கல்வெட்டியல், ஓலைச்சுவடியியல் மற்றும் தொல்லியல் சார்ந்த ஆவணத் தேடலுக்குரிய ஆய்வுமனப்பான்மையுடன், இலக்கியங்களை அணுகுதல்.
3. தமிழின் வளர்ச்சித் துறையாகிய, 'அறிவியல் தமிழ்' ; 'இணைய தமிழ்' குறித்த பன்னோக்கு அணுகுமுறையிலான ஆய்வுச் சிந்தனை மேம்பாடு.
4. வேலைவாய்ப்புக்குரிய சுயதிறன் மேம்பாட்டுடன், படைப்பாக்கத்திறன் மேம்பாடும் பெற்றிருத்தல் .
5. சமுதாய மற்றும் வாழ்வியல் மதிப்புகளைப் பேணுவதற்குக் கருவியாக இலக்கியங்களை நாடுகின்ற மனப்பான்மை வளர்ச்சி.
6. மொழிபெயப்புத் துறைசார்ந்த வேலைவாய்ப்புத் திறன் பெற்றிருத்தல்

அலகு – I : பக்தி இலக்கியம்

(10 மணிநேரம்)

சைவ, வைணவ இலக்கியங்கள் - தோற்றம் ,வளர்ச்சி, வரலாறு.

1. சைவம் -பெரியபுராணம் - திருமூலநாயனார் புராணம்.
2. வைணவம் - பெரியாழ்வார் திருமொழி: 10 பாடல்கள்.

அலகு – II : சங்கஇலக்கியம் :

(15 மணிநேரம்)

சங்க இலக்கியங்கள் அறிமுகம்

அ).எட்டுத்தொகை

நற்றிணை : பிரசம் கலந்த – பாலை -110
குறுந்தொகை : கருங்கட்டாக் கலை – குறிஞ்சி- 69
ஐங்குறுநூறு : நெய்தல்-தொண்டிப்பத்து:
திரைஇமிழ் இன்னிசை-171

பதிற்றுப்பத்து : சிதைந்தது மன்ற - 27

பரிபாடல் : பரிபாடல் திரட்டு-மதுரை நகர்ச்சிறப்பு -உலகம் ஒரு நிறையாத்தான்-6, மாயோன் கொப்பூழ்-7, செய்யாட்டு இழைத்த-9, கார்த்திகை காதில்-10, ஈவாரைக் கொண்டாடி-11.

கலித்தொகை : சுடர்தொடிகேளாய்: குறிஞ்சிக்கலி- 36

அகநானூறு : அன்னாய் வாழி வேண்டன்னை - குறிஞ்சி - 48

புறநானூறு : யாதும் ஊரே யாவருங் கேளிர் -பொதுவியல்- 192

ஆ). பத்துப்பாட்டு

திருமுருகாற்றுப்படை - பழமுதிர்ச்சோலையின் சிறப்பு

முருகன் இருப்பிடங்கள் - 'சிறுதினை மலரொடு' என்பதிலிருந்துதொடங்கி,

'அறிந்தவாறே' என்பது வரையிலான தொடர்கள்: 218-249.

முருகன் அருள்புரிதல் - 'தெய்வம் சான்ற' என்பதிலிருந்து தொடங்கி,

'நல்குமதி' என்பது வரையிலான தொடர்கள்: 286-295.

அலகு - III :காப்பியம்

(6 மணிநேரம்)

சிலப்பதிகாரம்:

மங்கல வாழ்த்துப் பாடல்: (21-29) - கண்ணகியின் சிறப்பு:

'நாகநீள் நகரொடு' என்பதிலிருந்து தொடங்கி,

'கண்ணகி என்பாண் மன்னோ' என்பது வரையிலான தொடர்கள்.

நடுகற்காதை: (207-234)- சேரன் செங்குட்டுவன் கண்ணகிக்குக் கோயில் எடுத்தல்:

'அருந்திறலரசர்' என்பதிலிருந்து தொடங்கி, 'மன்னவரேறென்' என்பது வரையிலான தொடர்கள்.

வாழ்த்துக்காதை: (482-485)- செங்குட்டுவனுக்குக் கண்ணகி காட்சியளித்தல்: 'என்னே'

என்பதிலிருந்து தொடங்கி, 'விசும்பில் தோன்றுமால்' என்பது வரையிலான தொடர்கள்.

வழக்குரை காதை:பத்தினிப் பெண்டிர் எழுவர் கதை: 'நீர்வார் கண்ணை' என்பதிலிருந்து

தொடங்கி, 'புகாரென் பதியே' என்பது வரையிலான தொடர்கள்.

வஞ்சினமாலை: 'வன்னி மரமும்' என்பதிலிருந்து தொடங்கி, 'பதிப்பிறந்தேன்' என்பது

வரையிலான தொடர்கள்.

அலகு - IV :சிறுகதை

(10 மணிநேரம்)

1. குளத்தங்கரை அரசமரம் - வ.வே.சு.ஐயர்

2. காட்டில் ஒரு மான் - அம்பை

3. நாற்காலி - கி.ராஜநாராயணன்

4. நகரம் - சுஜாதா

அலகு- V :மொழிப்பயிற்சி

(7 மணிநேரம்)

படைப்பிலக்கியப் பயிற்சிகள் (கதை, கவிதை, கட்டுரை, உரைநடை)மொழிபெயர்ப்பு

பாடநூல்:கற்பகச்சோலை - தமிழ்ஏடு.கற்பகம்பல்கலைக்கழகத்தமிழ்த்துறை வெளியீடு.

Instruction Hours/week:L: 4 T:0 P:0Marks: Internal:40 External: 60 Total:100**End Semester Exam: 3 hrs****Course Objectives**

This course enables the students to learn

- The Concept of Fourier analysis and solving boundary value problems.
- Techniques of Fourier and Laplace transform
- To solve differential equations.
- To Solve integration equation
- To Solve laplacian equation
- Numerical techniques of differentiation and integration.

Course Outcomes (COs)

On successful completion of this course, the students will be able to

1. Appreciate the physical significance of Fourier series
2. Understood the mathematical principles on transforms.
3. Apply mathematical foundation to formulate and solve problems arising in physics
4. Synthesize numerical techniques for practical problems
1. Solving integration equation
5. Solving laplacian equation

UNIT I

Fourier series: Definition – Finding Fourier coefficients for a given periodic function with period 2π – Odd and Even functions – Half Range Series

UNIT II

Fourier Transforms: Definition of Fourier Transform-Properties of Fourier Transform- Inverse Fourier transform-Convolution theorem-Finite Fourier Sine &Cosine Transform –Parseval's theorem.

UNIT III

Laplace Transforms: Definition of Laplace Transform - Properties of Laplace Transform, Inverse Laplace Transform. Application of Laplace Transform.

UNIT IV

Differential Equations: Types of Linear differential equations with constant coefficients – Simultaneous differential equations with constant coefficient.

UNIT V

Numerical methods: Solving simultaneous equations–Gauss Elimination method, Gauss Jordan method, Gauss – Seidel method. Numerical Integration – Trapezoidal Rule, Simpson’s Rule.

TEXT BOOKS

1. Sastry .S.S.,2009. Engineering Mathematics, PHI learning Pvt. Ltd, New Delhi(For Unit I, II, III & IV)
2. Kandasamy. P., K.Thilagavathy., and K.Gunavathy., 2003. Numerical methods, S. Chand & company Ltd, New Delhi (For Unit V)

REFERENCES

- 1.Singaravelu.A.,2011,Engineering Mathematics Vol I &Vol II Meenakshi Publications, Arpakkam.
- 2.Venkataraman.M.K., 2001. Engineering Mathematics Vol II, National Publishing Company, Chennai.
3. ManicavachagomPillay. T.K.S.Narayanan,2000, “Calculus Vol II”, S. Viswanathan (Printers and Publishers), PVT., LTD.
4. Sundaram.V, R. Balasubramaniam, And K.A.Lakshminarayanan, 2001, Engineering Mathematics – Vol III, Vikas Publishing House PVT., LTD, New Delhi.

**19CHU201 PHYSICAL CHEMISTRY II: Chemical
Thermodynamics and its applications****5H 5C****Instruction Hours/week:L: 5 T:0 P:0Marks: Internal:40 External: 60 Total:100****End Semester Exam: 3 hrs****Course Objectives**

- To outline the basics of chemical thermodynamics and the concept of first law of Thermodynamics.
- To discuss the knowledge about the thermo chemistry and to explain about the 2nd law of Thermodynamics.
- To explain the concepts of third law of thermodynamics and systems of variable composition.
- To explain about the usage of chemical thermodynamics in chemical equilibrium.
- To recognise the forces which drive the chemical reactions in forward direction and the concept of the interchange of energy in a system.
- To paraphrase a knowledge about solutions and colligative properties.

Course Outcomes

1. Apply the basic concepts of calculus to concepts in chemistry.
2. Describe the Three Laws of Thermodynamics and their development.
3. Use the Maxwell equations and other thermodynamic relations to compute thermodynamic quantities from thermodynamic data tables.
4. Derive the relationships between thermodynamic quantities; Interpret phase diagrams and explain phase equilibria in terms of chemical potentials.
5. Recognise the forces which drive the chemical reactions in forward direction and the concept of the interchange of energy in a system.
6. Explain the use of electrical energy for initiating chemical reactions and also how chemical reactions can be utilized to produce electrical energy, and the basic principle used in the formation of cells and batteries.

UNIT I

Chemical Thermodynamics: Intensive and extensive variables; state and path functions; isolated, closed and open systems.

First law: Concept of heat, Q, work, W, internal energy, U, and statement of first law; enthalpy, H, relation between heat capacities, calculations of Q, W, ΔU and ΔH for reversible, irreversible and free expansion of gases (ideal and Van der Waals) under isothermal and adiabatic conditions.

UNIT II

Thermochemistry: Heats of reactions: standard states; enthalpy of formation and enthalpy of combustion and its applications; effect of temperature (Kirchhoff's equations) and pressure on enthalpy of reactions.

Second Law: Concept of entropy; thermodynamic scale of temperature, statement of the second law of thermodynamics. Calculation of entropy change for reversible and irreversible processes.

UNIT III

Third Law: Statement of third law, concept of residual entropy, calculation of absolute entropy of molecules. Free Energy Functions: Gibbs and Helmholtz energy; variation of S, G, A with T, V, P; Free energy change and spontaneity. Relation between Joule-Thomson coefficient and other thermodynamic parameters; inversion temperature; Gibbs-Helmholtz equation; Maxwell relations; thermodynamic equation of state.

Systems of Variable Composition: Partial molar quantities, dependence of thermodynamic parameters on composition; Gibbs Duhem equation, chemical potential of ideal mixtures, change in thermodynamic functions in mixing of ideal gases.

UNIT IV

Chemical Equilibrium: Criteria of thermodynamic equilibrium, degree of advancement of reaction, chemical equilibria in ideal gases. Thermodynamic derivation of relation between Gibbs free energy of reaction and reaction quotient. Equilibrium constants and their quantitative dependence on temperature, pressure and concentration (Le Chatelier Principle, Quantitatively). Free energy of mixing and spontaneity. Equilibrium between ideal gases and a pure condensed phase.

UNIT V

Solutions and Colligative Properties: Dilute solutions; lowering of vapour pressure, Raoult's and Henry's Laws and their applications. Thermodynamic derivation using chemical potential to derive relations between the four colligative properties [(i) relative lowering of vapour pressure, (ii) elevation of boiling point, (iii) Depression of freezing point, (iv) osmotic pressure] and amount of solute. Applications in calculating molar masses of normal, dissociated and associated solutes in solution.

Suggested Readings

1. Peter, A. & Paula, J. de. (2011). Physical Chemistry. 9th Ed. Oxford University Press.
2. Castellan, G. W. (2004). Physical Chemistry. 4th Ed. Narosa.
3. Madan, R. L. (2015). Chemistry for Degree Students, S. Chand & Company Pvt. Ltd. Ram Nagar, New Delhi.
4. Engel, T. & Reid, P. (2012). Physical Chemistry. 3rd Ed. Prentice-Hall
5. McQuarrie, D. A. & Simon, J. D. (2004). New Delhi: Molecular Thermodynamics Viva Books Pvt. Ltd.
6. Assael, M. J., Goodwin, A. R. H., Stamatoudis, M., Wakeham, W. A. & Will, S. (2011). Commonly Asked Questions in Thermodynamics. NY : CRC Press.
7. Levine, I. N. (2010). Physical Chemistry. 6th Ed. Tata Mc Graw Hill. •
8. Metz, C. R. (2006). 2000 solved problems in chemistry. Schaum Series

**19CHU203 ORGANIC CHEMISTRY II:5H 5C
containing Functional Groups****Semester-II
Oxygen****Instruction Hours/week:L:5 T:0 P:0Marks: Internal:40 External: 60 Total:100
End Semester Exam: 3 hrs****Course Objectives**

To describe the students a knowledge on

- Chemistry of halogenated compounds like alkyl halides
- Chemistry of aryl halides and their uses
- The preparation, properties and relative reactivity of alcohols and phenols
- Preparation, properties and standard reactions of carbonyl compounds.
- Chemistry of Organometallic compounds, Ethers and Epoxides and Addition reactions
- Chemistry of carboxylic acids and their derivatives.

Course Outcomes (CO's)

The students will able to

1. Explain the chemistry of alkyl halides .
2. Explain the chemistry of aryl halides.
3. Contrast the preparation, properties and relative reactivity of alcohols and phenols
4. Summarise Preparation, properties and standard reactions of carbonyl compounds
5. Discuss the preparations, reactions and applications of epoxides, ethers and organometallic compounds
6. List the preparations and properties of carboxylic acid and its derivatives.

UNIT I**Chemistry of Halogenated Hydrocarbons:**

Alkyl halides: Methods of preparation and properties, nucleophilic substitution reactions – SN1, SN2 and SNi mechanisms with stereochemical aspects and effect of solvent; nucleophilic substitution vs. elimination.

Aryl halides: Preparation (including preparation from diazonium salts) and properties, nucleophilic aromatic substitution; SNAr, Benzyne mechanism.

Relative reactivity of alkyl, allyl, benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.

UNIT II**Alcohols, Phenols:**

Alcohols: preparation, properties and relative reactivity of 1°, 2°, 3° alcohols, Bouvaelt-Blanc Reduction; Oxidation of diols by periodic acid and lead tetraacetate, Pinacol-Pinacolone rearrangement;

Phenols: Preparation and properties; Acidity and factors affecting it, Ring substitution reactions, Reimer–Tiemann and Kolbe's–Schmidt Reactions, Fries and Claisen rearrangements with mechanism;

UNIT III

Carbonyl Compounds:

Structure, reactivity, preparation and properties; Nucleophilic additions, Nucleophilic addition-elimination reactions with ammonia derivatives with mechanism; Mechanisms of Aldol and Benzoin condensation, Knoevenagel condensation, Claisen-Schmidt, Perkin, Cannizzaro and Wittig reaction, Beckmann and Benzil-Benzilic acid rearrangements, haloform reaction and Baeyer Villiger oxidation, α – substitution reactions, oxidations and reductions (Clemmensen, Wolff-Kishner, LiAlH_4 , NaBH_4 , MPV, PDC)

UNIT IV

Organometallic compounds, Ethers and Epoxides and Addition reactions

Organometallic compounds of Mg (Grignard reagent) – Use in synthesis of organic compounds. *Ethers and Epoxides*: Preparation and reactions with acids. Reactions of epoxides with alcohols, ammonia derivatives and LiAlH_4

Addition reactions of α , β - unsaturated carbonyl compounds: Michael addition. Active methylene compounds: Keto-enol tautomerism. Preparation and synthetic applications of diethyl malonate and ethyl acetoacetate.

UNIT V

Acids and their Derivatives:

General methods of preparation, physical properties and reactions of monocarboxylic acids, effect of substituents on acidic strength. Typical reactions of dicarboxylic acids, hydroxy acids and unsaturated acids.

Preparation and reactions of acid chlorides, anhydrides, esters and amides; Comparative study of nucleophilic substitution at acyl group -Mechanism of acidic and alkaline hydrolysis of esters, Claisen condensation, Dieckmann and Reformatsky reactions, Hofmann- bromamide degradation and Curtius rearrangement.

Suggested Readings:

1. Morrison, R. N. & Boyd, R. N. (2012). *Organic Chemistry*. India: Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Madan, R. L. (2015). *Chemistry for Degree Students*, S. Chand & Company Pvt. Ltd. Ram Nagar, New Delhi-110055
3. Soni, P.L. and Chawla, H.M. (2003) *Text book of Organic Chemistry*. Sulthan Chand & Sons, Educational publishers, New Delhi.
4. Finar, I. L. (2013). *Organic Chemistry*. Volume 1. Edition-VI. Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
5. Graham Solomons, T.W. (2012). *Organic Chemistry*. John Wiley & Sons, Inc.
6. Jain M.K. & Sharma S.C. (2015). *Modern Organic Chemistry*, 4th Edition, Vishal publishing Co New Delhi.

Instruction Hours/week:L: 0 T:0 P:2Marks: Internal:40 External: 60 Total:100**End Semester Exam: 3 hrs**

Course Objectives

This course enables the students to learn

- To solve simultaneous linear algebraic equations using various methods.
- To evaluate definite integrals using numerical techniques.
- Problem-solving through (computer language) programming.
- Numerical Integration – Simpson's one third rule
- Numerical Integration – Simpson's three eighth rule
- Numerical Integration – Trapezoidal rule

Course Outcomes (COs)

On successful completion of this course, the student will be able to

1. Familiarize with the programming environment for numerical methods.
2. Develop proficiency in skills to solve the algebraic equations.
3. Evaluate the definite integrals using computer programming techniques
4. Numerical Integration – Simpson's one third rule
5. Numerical Integration – Simpson's three eighth rule
6. Numerical Integration – Trapezoidal rule

List of Practicals

1. Solution of simultaneous linear algebraic equations – Gauss Elimination method
2. Solution of simultaneous linear algebraic equations – Gauss Jordan method
3. Solution of simultaneous linear algebraic equations – Gauss Jacobi method
4. Solution of simultaneous linear algebraic equations – Gauss Seidal method
5. Numerical Integration – Simpson's one third rule
6. Numerical Integration – Simpson's three eighth rule
7. Numerical Integration – Trapezoidal rule

**19CHU212 CHEMICAL THERMODYNAMICS AND 2H 1C
ITS APPLICATIONS- PRACTICAL****Instruction Hours/week:L: 0 T:0 P:2Marks: Internal:40 External: 60 Total:100****End Semester Exam: 3 hrs****Course Objectives**

The Students have a present knowledge

- To measure the heat capacity of a calorimeter
- To determine the enthalpy of neutralisation.
- To determine the ionisation of solution.
- To determine the enthalpy of hydration of salt.
- To measure the integral enthalpy of solution
- To determine the basicity of a diprotic acid

Course Outcomes (CO's)

It enables the students calculate

1. The heat capacity of a calorimeter
2. The enthalpy of neutralisation,
3. Calculated the ionisation of solution.
4. Calculated the enthalpy of hydration of salt.
5. The integral enthalpy of solution
6. The basicity of a diprotic acid

Thermochemistry:

- (a) Determination of heat capacity of a calorimeter for different volumes using (i) change of enthalpy data of a known system (method of back calculation of heat capacity of calorimeter from known enthalpy of solution of sulphuric acid or enthalpy of neutralization), and (ii) heat gained equal to heat lost by cold water and hot water respectively
- (b) Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
- (c) Determination of the enthalpy of ionization of ethanoic acid.
- (d) Determination of integral enthalpy (endothermic and exothermic) solution of salts.
- (e) Determination of basicity of a diprotic acid by the thermochemical method in terms of the changes of temperatures observed in the graph of temperature versus time for different additions of a base. Also calculate the enthalpy of neutralization of the first step.
- (f) Determination of enthalpy of hydration of salt.
- (g) Study of the solubility of benzoic acid in water and determination of ΔH .

Suggested Readings:

1. Khosla, B. D.; Garg, V. C. & Gulati, A. (2011). *Senior Practical Physical Chemistry*. New Delhi: R. Chand & Co.
2. Athawale, V. D. & Mathur, P. (2011). *Experimental Physical Chemistry*. New Delhi: New Age International.

Semester-II**19CHU 213 OXYGEN CONTAINING FUNCTIONAL GROUPS - PRACTICAL**

Instruction Hours/week: L: 0 T: 0 P: 2 Marks: Internal: 40 External: 60 Total: 100**End Semester Exam: 3 hrs****Course Objectives**

The Students have a present knowledge

- To analyse the organic functional groups like alcohols, phenols carbonyl and carboxylic acid groups
- To demonstrate the preparations of organic compounds by acylation reactions
- To demonstrate the preparations of organic compounds by benzylation reactions.
- To carry out the iodoform reactions and selective reductions.
- To prepare semicarbazone derivatives of ketones
- To prepare S-Benzylisothiuronium salt of aromatic acids.

Course Outcomes

The student know to classifying the

1. Identification the organic functional groups like alcohols, phenols carbonyl and carboxylic acid groups
2. Preparation organic compounds by acylation reactions
3. Preparation organic compounds by benzylation reactions.
4. Iodoform reactions and selective reductions.
5. Preparations semicarbazone derivatives of ketones
6. Preparations S-Benzylisothiuronium salt of aromatic acids.

Experiments

1. Functional group tests for alcohols, phenols, carbonyl and carboxylic acid group.
2. Organic preparations:
 - i. Acetylation of one of the following compounds: amines (aniline, o-, m-, p- toluidines and o-, m-, p-anisidine) and phenols (β -naphthol, vanillin, salicylic acid) by any one method:
 - a. Using conventional method.
 - b. Using green approach
 - ii. Benzoylation of one of the following amines (aniline, o-, m-, p- toluidines and o-, m-, p-anisidine) and one of the following phenols (β -naphthol, resorcinol, p- cresol) by Schotten-Baumann reaction.
 - iii. Oxidation of ethanol/ isopropanol (Iodoform reaction).
 - iv. Selective reduction of meta dinitrobenzene to m-nitroaniline.
 - v. Hydrolysis of amides and esters.
 - vi. Semicarbazone of any one of the following compounds: acetone, ethyl methyl ketone, cyclohexanone, benzaldehyde.
 - vii. S-Benzylisothiuronium salt of one each of water soluble and water insoluble acids (benzoic acid, oxalic acid, phenyl acetic acid and phthalic acid).
 - viii. Aldol condensation using either conventional or green method.

The above derivatives should be prepared using 0.5-1g of the organic compound. The solid samples must be collected and may be used for recrystallization and melting point.

Suggested Readings

1. Mann, F.G. & Saunders, B.C.(2009). *Practical Organic Chemistry*. Pearson Education.
2. Furniss, B.S., Hannaford, A.J., Smith, P.W.G. & Tatchell, A.R. (2012). *Practical Organic Chemistry*. 5th Ed., Pearson.
3. Veeraiyan V, Venkateswaran R, and Vaithiyalingam A.R. (2015). *Basic Principles of Practical Chemistry*, S. Chand & Sons Ltd.
4. Raj K. Bansal, (2012). *Laboratory Manual of Organic Chemistry*, New Age International Publishers (P) Ltd.
5. Thomas A.O. (2003). *Practical Chemistry for B.Sc Main Students*, Scientific Book Centre, Cannore-1, Kerala.
6. Ahluwalia, V.K. & Aggarwal, R. (2000). *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*. University Press.
7. Ahluwalia, V.K. & Dhingra, S. (2000). *Comprehensive Practical Organic Chemistry: Qualitative Analysis*. University Press.

19AEC201	ENVIRONMENTAL STUDIES	Semester-II 3H 3C
Instruction Hours/week:L: 3 T:0 P:0	Marks: Internal: 40 External: 60 Total:100	End Semester Exam: 3 hrs

Course Objectives

It enables the students to

- The fundamental terms and definitions of environment
- Recall the Renewable and Non-renewable Resources.
- Quote the Biodiversity and Its Conservation
- Outline about Environmental Pollution
- Discuss the disaster management
- Discuss the Social Issues and the Environment

Course outcomes (CO's)**The students know about the explanation of**

1. Fundamental terms and definitions of environment
2. Renewable and Non-renewable Resources.
3. Biodiversity and Its Conservation
4. Environmental Pollution
5. Gained knowledge about disaster management
6. Social Issues and the Environment

UNIT-I

Environment Definition, scope and importance, components, Ecosystem Definition, Concept, Scope, importance, Structure and functions of ecosystem. Energy flow, Ecological succession Food chains and food webs. Classification of ecosystem.

UNIT II: Natural Resources**Renewable and Non-renewable Resources:**

Natural resources and associated problems. Forest resources, Water resources, Mineral resources, Food resources, Energy resources, Land resources: Use and over-utilization, exploitation. Role of an individual in conservation of natural resources. Equitable use of resources for sustainable lifestyles. Fire accidents and prevention.

UNIT III: Biodiversity and Its Conservation

Introduction, definition: genetic, species and ecosystem diversity. Biogeographical classification of India. Value of biodiversity: consumptive use, productive use, social, ethical, aesthetic and option values. Biodiversity at global, National and local levels. India as a mega-diversity nation. Hot-spots of biodiversity. Threats to biodiversity: habitat loss, poaching of wildlife, man-wildlife conflicts. Endangered and endemic species of India. Conservation of biodiversity: in-situ and ex-situ conservation of biodiversity.

UNIT IV: Environmental Pollution

Definition, Causes, effects and control measures of Air pollution, Water pollution, Soil pollution, Marine pollution, Noise pollution, Thermal pollution, Nuclear hazards, Solid waste management: Causes, effects and control measures of urban and industrial wastes. Role of an individual in prevention of pollution. Pollution case studies. Disaster management: Floods, earthquake, cyclone and landslides.

UNIT V: Social Issues and the Environment

From unsustainable to sustainable development. Urban problems related to energy. Water conservation, rain water harvesting, watershed management. Resettlement and rehabilitation of people; its problems and concerns. Environmental ethics: Issues and possible solutions. Climate change, global warming, acid rain, ozone layer depletion, nuclear accidents and holocaust. Case studies. Wasteland reclamation. Consumerism and waste products. Environment Protection Act. Air (Prevention and Control of Pollution) Act. Water (Prevention and Control of Pollution) Act. Wildlife Protection Act. Forest Conservation Act. Issues involved in enforcement of environmental legislation. Public awareness. Population growth, variation among nations. Population explosion—Family Welfare Programme. Environment and human health. Human rights. Value education. HIV/AIDS. Women and Child Welfare. Role of Information Technology in environment and human health.

Suggested Readings:

1. Tripathy, S.N. & Sunakar Panda. (2004). *Fundamentals of Environmental Studies*. 2nd Edition. New Delhi: Vrianda Publications Private Ltd.
2. Arvind Kumar. (2004). *A Textbook of Environmental Science*. New Delhi: APH Publishing Corporation.
3. Verma P.S., & Agarwal, V.K. (2001). *Environmental Biology : Principles of Ecology*. New Delhi: S.Chand and Company Ltd.
4. Anubha Kaushik, C.P. & Kaushik, (2004). *Perspectives in Environmental Studies*. New Delhi: New Age International Pvt. Ltd. Publications.
5. Singh, M.P., Singh, B.S. & Soma S. Dey, (2004). *Conservation of Biodiversity and Natural Resources*. Delhi: Daya Publishing House.
6. Daniel B. Botkin & Edward A. Keller. (1995). *Environmental Science*. New York: John Wiley and Sons, Inc.
7. Uberoi, N.K., (2005). *Environmental Studies*, New Delhi, India: Excel Books Publications.

19CHU301	Semester-III PHYSICS I	4H 4C
Instruction Hours/week:L: 4 T:0 P:0	Marks: Internal:40 External: 60 Total:100	End Semester Exam:3 hrs.

Course Objectives:

- To understand basic theories and experiments in Physics.
- To understand the fundamentals of physics.
- To educate and motivate the students in the field of science
- To Know about analog electronics
- To learn about amplifiers
- To study about digital electronics

Course Outcomes:

1. Students will demonstrate proficiency in mathematics and the mathematical concepts to understand physics.
2. Students will design and conduct an experiment (or series of experiments) demonstrating their understanding of the scientific method and processes.
3. Students will demonstrate an understanding of the analytical methods required to interpret and analyze results and draw conclusions as supported by their data.
4. Knowledge about analog electronics
5. Learnt about amplifiers
6. Study about digital electronics

UNIT – I**MODERN PHYSICS**

De Broglie's concept of matter waves- De Broglie's wavelength –Characteristics of De Broglie's matter waves- calculation of De Broglie's wavelength of material particles like electrons – experimental study of matter waves-Thomson's experiment

UNIT – II**ANALOG ELECTRONICS**

Construction, characteristics and applications of Zener diode, Photo diode, Light emitting diode (LED); working, efficiency, ripple factor and advantages of a full wave rectifier-Qualitative analysis of a common emitter amplifier; Phase reversal of the output voltage; Advantage of common emitter amplification circuit.

UNIT - III**AMPLIFIERS**

Circuit symbol polarity conventions and virtual ground or summing point of an operational amplifier; characteristics of an ideal operational amplifier; amplifier as an adder, subtractor, differentiator and integrator.

UNIT – IV**DIGITAL ELECTRONICS**

Number systems-Binary Octal-Hexa decimal-ASCII and EBCDIC-Redundant coding for error detection and correction. Basic logic design using digital integrated circuits. Truth tables,

Boolean algebra, Simple arithmetic circuits-exclusive half adder-full adder-half subtractor, full subtractor. NAND AND NOR As Universal Building Block-De Morgan's theorem and its proof.

UNIT –V

OPTICS

Reflection – Refraction – Snell's law – Total internal reflection – Interference – Diffraction – Polarisation – Coherence

Suggested Readings

1. Murugesan. R., Modern Physics, S.Chand & CO, New Delhi
2. Aruldas G. and P.Rajagopal, 'Modern Physics', Printice Hall of India, New Delhi, 2009
3. Rajam. J.B., Atomic Physics, S.Chand & Co, New Delhi.
4. Gupta and Kumar, 2000, Solid State Physics - Pragati Prakashan, Meerut.
5. Kittel. C., 1996, Introduction to Solid State Physics, 7TH Edition, John Willey & sons, New Delhi.
6. Dekkar. A.J. , 1900, Solid State Physics - Macmillan India Ltd., New Delhi.

19CHU302

INORGANIC CHEMISTRY III:

Coordination Chemistry

4H 4C

Instruction Hours/week:L:40 T:0 P:0 Marks: Internal:40 External: 60 Total:100

End semester Exam:3 hrs

Course Objectives

The students should be able

- To discuss the key features of coordination compounds,
- Understand the nomenclature, isomerism and types in coordination compounds.
- To describe the various theories to explain the characteristics of coordination compounds.
- To contrast the nature of transition elements and their compounds.
- To contrast about the occurrence, preparation and properties of Lanthanides and actinides.
- To discuss about the fundamentals of Inorganic reaction mechanisms.

Course Outcomes

The students have gained knowledge to summarise

1. Recognise the role played by transition metal complexes in Inorganic Chemistry.
2. Understand the nomenclature, isomerism and types in coordination compounds.
3. Describe the structure and bonding theories, electronic and magnetic properties of the transition metal complexes and their kinetic studies.
4. Explain the theories of bonding in coordination compounds and their experimental behaviour.
5. Recognise and explain the interaction of metal ions with biological ligands.
6. Explain the role of Inorganic “substances” in living systems and the use of metal ions in medicinal therapy and diagnosis.

UNIT I**Coordination Chemistry I:**

IUPAC nomenclature of coordination compounds, isomerism in coordination compounds. Stereochemistry of complexes with 4 and 6 coordination numbers. Chelate effect, polynuclear complexes, Labile and inert complexes.

UNIT II**Coordination Chemistry II:**

Werner's theory, valence bond theory (inner and outer orbital complexes), electroneutrality principle and back bonding. Crystal field theory, measurement of $10 Dq$ (Δ_o), CFSE in weak and strong fields, pairing energies, factors affecting the magnitude of $10 Dq$ (Δ_o , Δ_t). Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry Jahn-Teller theorem, square planar geometry. Qualitative aspect of Ligand field and MO Theory.

UNIT III

Transition Elements:

General group trends with special reference to electronic configuration, colour, variable valency, magnetic and catalytic properties, ability to form complexes. Stability of various oxidation states and e.m.f. (Latimer diagrams) Different between the first, second and third transition series. Chemistry of Cr, Mn, Fe and Co in various oxidation states with special reference to the following compounds: peroxo compounds of chromium, potassium dichromate, potassium permanganate, potassium ferrocyanide, potassium ferricyanide, sodium nitroprusside and sodium cobaltinitrite.

UNIT IV

Lanthanides and Actinides:

Electronic configuration, oxidation states, colour, spectral and magnetic properties, lanthanide contraction, separation of lanthanides (ion-exchange method only).

Actinides: Occurrence, Preparation of elements, Electronic structure, Oxidation State and general properties. Thorium: Extraction of Thorium.

UNIT V

Inorganic Reaction Mechanism

Introduction to inorganic reaction mechanisms. Substitution reactions in square planar complexes, Trans- effect, theories of trans effect. Thermodynamic and Kinetic stability.

Suggested Readings

1. Purcell, K.F & Kotz, J.C. (1980). *An Introduction to Inorganic Chemistry*. W.B. Saunders Co.
2. Huheey, J.E. (1993). *Inorganic Chemistry*. Prentice Hall.
3. Cotton, F.A. & Wilkinson, G. (1999). *Advanced Inorganic Chemistry*. Wiley-VCH.
4. Greenwood, N.N. & Earnshaw A. (2006). *Chemistry of the Elements*. Butterworth-Heinemann.
5. Miessler, G. L. & Tarr, Donald A. (2009). *Inorganic Chemistry*. 3rd Ed. (adapted), Pearson.

Semester-III

19CHU303 PHYSICAL CHEMISTRY III:Phase equilibria and chemical kinetics 4H 4C**Instruction Hours/week:L: 4 T:0 P:0 Marks: Internal:40 External: 60 Total:100****End Semester Exam:3 hrs.****Course Objectives**

The students should be able

- To illustrate the phase equilibrium.
- Understand the Clacius-Clapeyron equation and its applications.
- To explain the theory behind three component systems
- To summarize about electrochemical cells and EMF measurements
- To discuss the applications of EMF measurements
- To contrast the fundamentals of surface chemistry

Course Outcomes

The students have gained knowledge to summarise

1. The concept of Phase equilibria and phase diagrams
2. Understood the Clacius-Clapeyron equation and its applications.
3. About three component systems and their characteristic properties
4. Different types of electrochemical cells and EMF measurements
5. Applictions of EMF measurements in determining thermodynamic properties
6. The basics of surface chemistry.

UNIT I

Phase Equilibria: Concept of phases, components and degrees of freedom, derivation of Gibbs Phase Rule for nonreactive and reactive systems; Clausius-Clapeyron equation and its applications to solid-liquid, liquid-vapour and solid-vapour equilibria, phase diagram for onecomponent systems (H_2O and S), with applications. Phase diagrams for systems of solid-liquid equilibria involving eutectic, congruent and incongruent melting points.

UNIT II

Three component systems: triangular plots, water-chloroform-acetic acid system. Binary solutions: Gibbs-Duhem-Margules equation, its derivation and applications to fractional distillation of binary miscible liquids (ideal and non ideal), azeotropes, lever rule, partial miscibility of liquids, CST, miscible pairs, steam distillation. Nernst distribution law: its derivation and applications.

UNIT III

Electrochemical Cells: Rules of oxidation/reduction of ions based on half-cell potentials, applications of electrolysis in metallurgy and industry. Chemical cells, reversible and irreversible cells with examples. Electromotive force of a cell and its measurement, Nernst

equation; Standard electrode (reduction) potential and its application to different kinds of half-cells. Electrochemical series and its applications.

UNIT IV

Application of EMF measurements in determining (i) free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values, using hydrogen, quinone-hydroquinone, glass and $\text{SbO/Sb}_2\text{O}_3$ electrodes. Concentration cells with and without transference, liquid junction potential; determination of activity coefficients and transference numbers. Qualitative discussion of potentiometric titrations (acid-base, redox, precipitation).

UNIT V

Surface chemistry: Physical adsorption, chemisorption, adsorption isotherms (Langmuir and Freundlich). nature of adsorbed state. Qualitative discussion of BET. The role of surface chemistry in chromatography (TLC and Column) and Gibb's adsorption isotherm.

Suggested Readings:

1. Peter Atkins & Julio De Paula. (2010). *Physical Chemistry*. 9th Ed. Oxford University Press.
2. Castellan, G. W. (2004). *Physical Chemistry*. 4th Ed. Narosa
3. McQuarrie, D. A. & Simon, J. D. (2004). *Molecular Thermodynamics*. New Delhi : Viva Books Pvt. Ltd. • Engel, T. & Reid, P. (2012). *Physical Chemistry*. 3rd Ed. Prentice-Hall
4. Assael, M. J., Goodwin, A. R. H., Stamatoudis, M., Wakeham, W. A. & Will, S. (2011). *Commonly Asked Questions in Thermodynamics*. NY : CRC Press.
5. Zundhal, S.S. (2011). *Chemistry concepts and applications*. Cengage India • Ball, D. W. (2012). *Physical Chemistry*. Cengage India.
6. Mortimer, R. G. (2009). *Physical Chemistry*. 3rd Ed. Elsevier: NOIDA, UP.
7. Levine, I. N. (2011). *Physical Chemistry*. 6th Ed. Tata McGraw-Hill.
8. Metz, C. R. (2009). *Physical Chemistry*. 2nd Ed. Tata McGraw-Hill.

19CHU311

PHYSICS I PRACTICAL

Semester-III
4H 2C

Instruction Hours/week:L: 0 T:0 P:4

Marks: Internal:40 External: 60 Total:100

End Semester Exam: 3 hrs

Course Objective

- To acquire basic understanding of laboratory technique and
- To educate and motivate the students in the field of Physics
- To allow the students to have a deep knowledge of fundamentals of optics.
- To work efficient in the Young modulus, rigidity modulus
- Refractive Index of a liquid prism-Spectrometer
- Thickness of a thin wire-Air wedge method

Course outcome

Students can able to

1. Perform basic experiments in mechanics and electricity and analyze the data.
2. Acquire engineering skills and Practical knowledge, which help the student in their everyday life.
3. Knowledge about the physical Principles and applications of Electronics.
4. Work efficiently in the Young modulus, rigidity modulus
5. Refractive Index of a liquid prism-Spectrometer
6. Thickness of a thin wire-Air wedge method

Any 8 Experiments

1. Young's Modulus-Non Uniform bending-Optic lever
2. Young's Modulus-Static cantilever
3. Rigidity modulus- Dynamic method
4. Acceleration due to gravity-Compound pendulum
5. Refractive Index of a liquid prism-Spectrometer
6. Refractive Index of a solid prism (I-d) curve-Spectrometer
7. Co-efficient of thermal conductivity-Lee's disc method
8. Wavelength of spectral lines -Grating-minimum deviation method-Spectrometer.
9. Characteristics of a Junction diode
10. μ of a lens-Newton's ring method
11. Thickness of a thin wire-Air wedge method
12. Frequency of tuning fork and density of solid and liquid – Melde's String

References:

1. Ouseph C.C., U.J. Rao and V. Vijayendran 2007, Practical Physics and Electronics, S.Viswanathan (Printers & Publishers) Pvt. Ltd., Chennai
2. Singh S.P., 2003, Advanced Practical Physics – 1, 13th Edition, Pragathi Prakashan, Meerut
3. Singh S.P., 2000, Advanced Practical Physics – 2, 12th Edition, Pragathi Prakashan, Meerut

Course Objectives

The student should be able to

- Explain the principle of gravimetric analysis
- To estimate the amount of nickel present in the NiDMG
- Prepare coordination complexes
- To measure the 10Dq by spectrophotometrically.
- Justify the properties of coordination complexes
- To synthesise the ligand transfer reaction by substitution method.

Course outcomes

The students have to

1. Determine metals like Ni, Cu and Fe using the principle of gravimetric analysis
2. Estimate the amount of nickel present in the NiDMG
3. Prepare coordination complexes
4. Measurement of 10 Dq by spectrophotometric method
5. Justify the properties of coordination complexes
6. Synthesis of ammine complexes of Ni(II) and its ligand exchange reactions (e.g. bidentate ligands like acetylacetone, DMG, glycine) by substitution method.

Gravimetric Analysis:

- i. Estimation of nickel (II) using Dimethylglyoxime (DMG).
- ii. Estimation of copper as CuSCN
- iii. Estimation of iron as Fe₂O₃ by precipitating iron as Fe(OH)₃.

Inorganic Preparations:

- i. Tetraamminecopper (II) sulphate, [Cu(NH₃)₄]SO₄.H₂O
- ii. Acetylacetonate complexes of Cu²⁺/Fe³⁺
- iii. Tetraamminecarbonatocobalt (III) nitrate
- iv. Potassium tri(oxalato)ferrate(III)

Properties of Complexes

- i. Measurement of 10 Dq by spectrophotometric method
- ii. Synthesis of ammine complexes of Ni(II) and its ligand exchange reactions (e.g. bidentate ligands like acetylacetone, DMG, glycine) by substitution method.

Suggested Readings

1. Vogel, A.I. (2002). *A text book of Quantitative Analysis*. ELBS.
2. Marr, G. & Rockett, B.W. (1972). *Practical Inorganic Chemistry*. Van Nostrand Reinhold.

Semester-III

19CHU313 PHASE EQUILIBRIA AND CHEMICAL KINETICS- 4H 2C
PRACTICAL

Instruction Hours/week:L: 0 T:0 P:4 Marks: Internal:40 External: 60 Total:100
End Semester Exam: 3 hrs

Course Objectives

It enables the students to Paraphrase the

- To Determine of critical solution temperature (CST) and
- To Determine of eutectic temperature
- To Determine distribution coefficients of two immisible solutions.
- To construct of the phase diagram using cooling curves or ignition tube method: a. simple eutectic and b. congruently melting systems.
- To apply their knowledge in Potentiometry to laboratory.
- To perform the potentiometric titrations.

Course Outcomes

The students able to determine,

1. Apply their knowledge in Phase equilibria
2. Determination of critical solution temperature (CST) and
3. Determination of eutectic temperature
4. Determination distribution coefficients of two immisible solutions.
5. Apply their knowledge in Potentiometry to laboratory.
6. Perform the titrations potentiometrically.

Phase Equilibria:

- I. Determination of critical solution temperature and composition at CST of the phenolwatersystem and to study the effect of impurities of sodium chloride and succinic acidon it.
- II. Phase equilibria: Construction of the phase diagram using cooling curves or ignition tube method: a. simple eutectic and b. congruently melting systems.
- III. Distribution of acetic/ benzoic acid between water and chloroform or cyclohexane.
- IV. Study the equilibrium of at least one of the following reactions by the distribution method:
 - (i) $I_2(aq) + I^-(aq) \rightarrow I_3(aq)$
 - (ii) $Cu^{2+}(aq) + nNH_3 \rightarrow Cu(NH_3)_n^{2+}$

Potentiometry:

- V. Perform the following potentiometric titrations:
 - i. Strong acid vs. Strong base
 - ii. Weakacid vs. Strong base.

- iii. Dibasic acid vs. Strong base
- iv. Potassium dichromate vs. Mohr's salt

Suggested Readings

1. Khosla, B. D., Garg, V. C. & Gulati, A. (2011). *Senior Practical Physical Chemistry*. 25. New Delhi: R. Chand & Co.
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. (2003). *Experiments in Physical Chemistry*. 8th Ed. McGraw-Hill: New York.
3. Halpern, A. M. & McBane, G. C. (2003). *Experimental Physical Chemistry*. 3rd Ed. New York: W. H. Freeman & Co.

		Semester-III
19CHU304A	PHARMACEUTICAL CHEMISTRY	3H 3C
Instruction Hours/week:L:03 T:0 P:0Marks: Internal:40 External: 60 Total:100		End Semester Exam:3hrs.

Course Objectives

The course enables the students to

- Perform the drug discovery process.
- To utilize the software to predict the ADMET.
- Build the synthesis of analgesic, antipyretic, anti-inflammatory agents
- Build the synthetic process of Central Nervous System and cardiovascular drugs.
- Restate the fermentation process
- Modify to prepare antibiotics and related compounds.

Course Outcome

The students have knowledge to create about the

1. Drug discovery
2. Utilization of the software using prediction of ADMET
3. Procedures to prepare analgesic, antipyretic, anti-inflammatory agents
4. Synthesis of Central Nervous System and cardiovascular drugs.
5. Fermentation process and preparation of antibiotics.
6. Modified the preparation of antibiotics and related compounds

UNIT 1

Drug discovery, design and development; Basic Retrosynthetic approach.ADMET properties, Lipinski's rule of five, Cheminformatics tools,Synthon,FGI.

UNIT II

Synthesis of the representative drugs of the following classes: analgesic agents, antipyretic agents, anti-inflammatory agents (Aspirin, paracetamol, Ibuprofen); antibiotics (Chloramphenicol);antibacterial and antifungal agents (Sulphonamides; Sulphanethoxazol, Sulphacetamide,Trimethoprim); antiviral agents (Acyclovir),

UNIT III

Synthesis of the representative drugs of the following classes: Central Nervous System agents (Phenobarbital,Diazepam),Cardiovascular (Glyceryl trinitrate), antileprosy (Dapsone), HIV-AIDS related drugs (AZT- Zidovudine).Blood Brain Barrier(BBB).

UNIT IV**Fermentation**

Aerobic and anaerobic fermentation. Production of Ethyl alcohol and citric acid,

UNIT V

Production of (i) Antibiotics; Penicillin, Cephalosporin, Chloromycetin and Streptomycin, (iii) Lysine, Glutamic acid, Vitamin B2, Vitamin B12 and Vitamin C.

Suggested Readings

1. Patrick, G.L.(1995). *Introduction to Medicinal Chemistry*. 65. UK: Oxford University Press
2. Hakishan, V.K. Kapoor,(1996). *Medicinal and Pharmaceutical Chemistry*, New Delhi: Vallabh Prakashan. Pitampura.
3. William O. Foye, Thomas L., Lemke & David A. William.(2008). *Principles of Medicinal Chemistry*. New Delhi: B.I. Waverly Pvt. Ltd.

Course Objectives

The course enables the student to gain knowledge in the mathematics and computer science to

- Interpret the Uncertainty in experimental techniques
- Statistical treatment
- Error analysis
- Summarise the types of algebraic operations
- Explain computer programming and to handle numeric data
- Illustrate the numerical modelling

Course Outcomes

1. Interpret the Uncertainty in experimental techniques and Statistical treatment
2. Under stood the knowledge of error analysis.
3. Formulate a set of calculations that can address a relevant research question;
4. Use one or several computer programs and extract useful information;
5. Write a research paper that describes methods, results, and interpretation;
6. Assess the meaning and validity of calculations that appear in the chemical literature.

UNIT I

Mathematics

Fundamentals, mathematical functions, polynomial expressions, logarithms, the exponential function, units of a measurement, interconversion of units, constants and variables, equation of a straight line, plotting graphs. Uncertainty in experimental techniques: Displaying uncertainties, measurements in chemistry, decimal places, significant figures, combining quantities. Uncertainty in measurement: types of uncertainties, combining uncertainties. Statistical treatment. Mean, standard deviation, relative error. Data reduction and the propagation of errors. Graphical and numerical data reduction. Numerical curve fitting: the method of least squares (regression).

UNIT II

Algebraic operations on real scalar variables (e.g. manipulation of Van der Waals equation in different forms). Roots of quadratic equations analytically and iteratively (e.g. pH of a weak acid). Numerical methods of finding roots (Newton-Raphson, binary – bisection, e.g. pH of a weak acid not ignoring the ionization of water, volume of a van der Waals gas, equilibrium constant expressions). Differential calculus: The tangent line and the derivative of a function, numerical differentiation (e.g., change in pressure for small change in volume of a

Vander Waals gas, potentiometric titrations). Numerical integration (Trapezoidal and Simpson's rule, e.g. entropy/enthalpy change from heat capacity data).

UNIT III

Computer programming:

Constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions. Elements of the BASIC language. BASIC keywords and commands. Logical and relative operators. Strings and graphics. Compiled versus interpreted languages. Debugging. Simple programs using these concepts. Matrix addition and multiplication. Statistical analysis.

UNIT IV

Introductory writing activities: Introduction to word processor and structure drawing (ChemSketch) software. Incorporating chemical structures, chemical equations, expressions from chemistry (e.g. Maxwell-Boltzmann distribution law, Bragg's law, van der Waals equation, etc.) into word processing documents.

Handling numeric data: Spreadsheet software (Excel), creating a spreadsheet, entering and formatting information, basic functions and formulae, creating charts, tables and graphs. Incorporating tables and graphs into word processing documents. Simple calculations, plotting graphs using a spreadsheet (Planck's distribution law, radial distribution curves for hydrogenic orbitals, gas kinetic theory- Maxwell-Boltzmann distribution curves as function of temperature and molecular weight), spectral data, pressure-volume curves of van der Waals gas (van der Waals isotherms), data from phase equilibria studies. Graphical solution of equations.

UNIT V

Numeric modelling: Simulation of pH metric titration curves. Excel functions LINEST and Least Squares. Numerical curve fitting, linear regression (rate constants from concentration time data, molar extinction coefficients from absorbance data), numerical differentiation

(e.g. handling data from potentiometric and pH metric titrations, pK_a of weak acid), integration (e.g. entropy/enthalpy change from heat capacity data).

Statistical analysis: Gaussian distribution and Errors in measurements and their effect on data sets. Descriptive statistics using Excel.

Suggested Readings

1. McQuarrie, D. A. (2008). *Mathematics for Physical Chemistry*. University Science Books
2. Mortimer, R. (2005). *Mathematics for Physical Chemistry*. 3rd Ed. Elsevier
3. Steiner, E. (1996). *The Chemical Maths Book*. Oxford University Press.
4. Yates, P. (2007). *Chemical calculations*. 2nd Ed. CRC Press.
5. Harris, D. C. (2007). *Quantitative Chemical Analysis*. 6th Ed. Freeman Chapters 3-5.
6. Levie, R. de. (2001). *How to use Excel in analytical chemistry and in general scientific data Analysis*. Cambridge Univ. Press 487 pages.
7. Noggle, J. H. (1985). *Physical chemistry on a Microcomputer*. Little Brown & Co.

8. Venit, S.M. (1996). *Programming in BASIC: Problem solving with structure and style*. Delhi :Jaico Publishing House.

B.Sc. Chemistry

2019-2020

Semester-III

19CHU314PHARMACEUTICAL CHEMISTRY - PRACTICAL 3H 1C

Instruction Hours/week:L:0 T:0 P:03Marks: Internal:40 External: 60 Total:100

End Semester Exam: 3hrs.

Course Objective

The course enables the student to

- Develop the synthesis of pharmaceutical drugs like aspirin
- Synthesis of magnesium bisilicate.
- Determine the melting point of aspirin
- Spectral characterization of aspirin
- Determine the melting point of antacid
- Spectral characterization of antacid

Course Outcome

The students restate the

1. Synthesis of pharmaceutical drugs like aspirin
2. Synthesis of magnesium bisilicate.
3. Determination of the melting point of aspirin
4. Spectral characterization of aspirin
5. Determine the melting point of antacid
6. Spectral characterization of antacid

Methodology

Practicals

1. Preparation of Aspirin and its analysis.
2. Preparation of magnesium bisilicate (Antacid).

Suggested Readings

1. Patrick G.L. (1995): *Introduction to Medicinal Chemistry*. UK:Oxford University Press.
2. Hakishan, V.K. Kapoor, (1996) *Medicinal and Pharmaceutical Chemistry*. New Delhi: VallabhPrakashan. Pitampura.
3. William O. Foye, Thomas L., Lemke, & David A. Williams. (2008). *Principles of Medicinal Chemistry*. New Delhi: B.I. Waverly Pvt. Ltd.

19CHU314B IT SKILLS FOR CHEMISTS- PRACTICAL3H 1C**Instruction Hours/week: L:0 T:0 P:3 Marks: Internal: 40 External: 60 Total:100****End Semester Exam: 3hrs****Course Objectives**

The course enables the student to

- Describe the rules and the methods to be followed in the computer programming.
- Describe the basic programme of curve fitting
- Describe the numerical differentiation and integration.
- Interpret Statistical analysis of the numeric data.
- Draw the chemical structure using software
- Understand the statistical significance testing.

Course Outcome

The students have to explain the

1. The rules and the methods to be followed in the computer programming.
2. the basic programme of curve fitting
3. The numerical differentiation and integration.
4. Interpretation of Statistical analysis of the numeric data.
5. Draw the chemical structure using software
6. Understand the statistical significance testing.

BASIC programs for curve fitting, numerical differentiation and integration (Trapezoidal rule, Simpson's rule), finding roots (quadratic formula, iterative, Newton-Raphson method). Structure drawing software.

Statistical significance testing: The *t* test. The *F* test.

Presentation: Presentation graphics

Suggested Readings

1. McQuarrie, D. A. (2008). *Mathematics for Physical Chemistry*. University Science Books
2. Mortimer, R. (2005). *Mathematics for Physical Chemistry*. 3rd Ed. Elsevier.
3. Steiner, E. (1996). *The Chemical Maths Book*. Oxford University Press. Yates, P. (2007). *Chemical calculations*. 2nd Ed. CRC Press.
4. Harris, D. C. (2007). *Quantitative Chemical Analysis*. 6th Ed. Freeman Chapters 3-5.
5. Levie, R. de. (2001). *How to use Excel in analytical chemistry and in general scientific data analysis*, Cambridge Univ. Press 487 pages.
6. Noggle, J. H. (1985). *Physical chemistry on a Microcomputer*. Little Brown & Co.
7. Venit, S.M. (1996). *Programming in BASIC: Problem solving with structure and style*. Delhi :Jaico Publishing House

19CHU401	PHYSICS-II	Semester-IV
		4H 4C
Instruction Hours/week:L:4 T:0 P:0 Marks: Internal:40 External: 60 Total:100		
End semester exam:3hrs		

Course Objectives:

- Many basic natural processes in nature can be explained by physics. So it is essential to know basic physics any science student. This paper is aimed at giving some insight into the basic physics, theory as well as experiment.
- To gain a knowledge of elasticity of solids.
- To understand the basics of surface tension
- To learn Eienstein's photoelectric effect.
- To knowledge about laser physics
- To gain a knowledge about solar physics.

Course Outcomes

The students have gained knowledge about

1. Basic natural processes of Physics
2. Gained about elasticity of solids.
3. Learned about Eienstein's photoelectric effect.
4. Understood the basics of surface tension.
5. Laser physics
6. Gained knowledge about solar physics

UNIT-I**ELASTICITY OF SOLIDS**

Elastic constants of an isotropic solid - Relations connecting them - Poisson's ratio - Bending of beams - Uniform and non-uniform bending - Bending moment of a bent beam - cantilever - Static and dynamic methods - Torsion in a wire - Rigidity modulus determination by Static and dynamic methods.

UNIT-II**SURFACE TENSION**

Surface tension and Surface energy- Pressure difference across a spherical surface- Pressure difference across a curved surface - Angle of contact - Angle of contact for water in a glass - Vapour pressure over a flat and curved surface - Variation of Surface tension with temperature - Jaeger's method - Quinke's method.

UNIT-III**MODERN PHYSICS:**

Photo electric effect – Einstein's photo electric equation –verification of Einstein's photo electric equation by Millikan's experiment – photo electric cells – applications

Nuclear physics : characteristics of nuclear forces – nuclear structure by liquid drop model – Binding energy – mass defect – particle accelerators – cyclotron and betatron
nuclear Fission and nuclear Fusion

UNIT-IV

LASER PHYSICS:

Purity of spectral lines – Coherence length and time – spontaneous and induced emissions – population inversion – meta stable state – conditions for laser actions – Ruby laser – Helium – neon laser – applications of lasers – Raman effect – Raman shift – stokes and anti stokes lines – Laser Raman Spectrometer.

UNIT-V

SOLAR PHYSICS:

solar constant – measurement of solar radiations by Pyroheliometer and Pyranometer – general applications of solar energy – flat–plate collector - box type cooker - solar water heaters – solar photo – voltaic cells – general applications of solar cells.

BOOKS FOR STUDY

Murugesan. R., Modern Physics, S.Chand & CO, New Delhi

Aruldas and P.Rajagopal, Modern Physics, Prentice Hall of India, New Delhi.

References:

1. Mathur. D.S., 2003, Elements of properties of matter - Shyamlal Charitable Trust, New Delhi.
2. Brijlal and N. Subramanyam, 2004, Properties of matter, S. Chand & Company, New Delhi.
3. Rai. G.D, Solar energy and its utilization, S.Chand & Co., New Delhi.
4. Rajam. J.B., Atomic Physics, S.Chand & Co, New Delhi.

Course Objectives

The course enables the students to

- Explain the types of conductance measurements and the factors affecting it
- Describe the ionic mobilities and the applications of conductance measurements
- Discuss the order and molecularity of reactions and the integrated rate expressions for different types of first order reactions.
- To knowledge about chemical kinetics
- Summarize the fundamentals of catalysis
- Restate the fundamentals of photochemistry.

Course Outcome

The students have to restated

1. The types of conductance measurements and the factors affecting it.
2. The ionic mobilities and the applications of conductance measurements
3. The order and molecularity of reactions and the integrated rate expressions for different types of first order reactions.
4. Gained knowledge about chemical kinetics.
5. The fundamentals of catalysis
6. The fundamentals of photochemistry.

UNIT I

Conductance: Quantitative aspects of Faraday's laws of electrolysis Arrhenius theory of electrolytic dissociation. Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Molar conductivity at infinite dilution. Kohlrausch law of independent migration of ions. Debye-Hückel-Onsager equation, Wien effect, Debye-Falkenhagen effect, Walden's rules.

UNIT II

Ionic velocities, mobilities and their determinations, transference numbers and their relation to ionic mobilities, determination of transference numbers using Hittorf and Moving Boundary methods. Applications of conductance measurement: (i) degree of dissociation of weak electrolytes, (ii) ionic product of water (iii) solubility and solubility product of sparingly soluble salts, (iv) conductometric titrations, and (v) hydrolysis constants of salts.

UNIT III

Chemical Kinetics: Order and molecularity of a reaction, rate laws in terms of the advancement of a reaction, differential and integrated form of rate expressions up to second order

reactions, experimental methods of the determination of rate laws, kinetics of complex reactions (integrated rate expressions up to first order only): (i) Opposing reactions (ii) parallel reactions and (iii) consecutive reactions and their differential rate equations (steady-state approximation in reaction mechanisms) (iv) chain reactions.

Unit IV

Temperature dependence of reaction rates; Arrhenius equation; activation energy. Collision theory of reaction rates, Lindemann mechanism, qualitative treatment of the theory of absolute reaction rates.

Catalysis: Types of catalyst, specificity and selectivity, mechanisms of catalyzed reactions at solid surfaces. Enzyme catalysis, Michaelis-Menten mechanism, acid-base catalysis.

Unit V

Photochemistry: Characteristics of electromagnetic radiation, Lambert-Beer's law and its limitations, physical significance of absorption coefficients. Laws of photochemistry, quantum yield, actinometry, examples of low and high quantum yields, photochemical equilibrium and the differential rate of photochemical reactions, photosensitized reactions, quenching. Role of photochemical reactions in biochemical processes, photostationary states, chemiluminescence.

Suggested Readings

1. Atkins, P.W & Paula, J.D.(2011). *Physical Chemistry*. 9th Ed. Oxford University Press.
2. Castellan, G. W.(2004). *Physical Chemistry*. 4th Ed. Narosa.
3. Mortimer, R. G. (2009). *Physical Chemistry*. 3rd Ed. Elsevier: NOIDA, UP.
4. Barrow, G. M.(2006). *Physical Chemistry*. 5th Ed. New Delhi : Tata McGraw Hill.
5. Engel, T. & Reid, P. (2012). *Physical Chemistry*. 3rd Ed. Prentice-Hall.
6. Rogers, D. W. (2010). *Concise Physical Chemistry*. Wiley.
7. Silbey, R. J., Alberty, R. A. & Bawendi, M. G. (2005). *Physical Chemistry*. 4th Ed. John Wiley & Sons, Inc.

Course Objectives

This course enables the students to

- Discuss the principle and the theory behind the UV spectroscopy.
- Discuss the principle and the theory behind the IR spectroscopy.
- Explain the principle and the theory behind the NMR spectroscopy.
- Summarize about the occurrence, classification and their biological importance carbohydrates
- Justify about the classification of dyes.
- Justify about polymers and their types, preparation and uses.

Course Outcome

The Student have gained knowledge about

1. The principle and the theory behind the UV spectroscopy.
2. The principle and the theory behind the IR spectroscopy.
3. The principle and the theory behind the NMR spectroscopy.
4. The occurrence, classification and their biological importance carbohydrates
5. The classification of dyes
6. Preparation ,types, properties and uses of polymers.

UNIT 1**Organic Spectroscopy**

General principles to absorption and emission spectroscopy.

UV Spectroscopy: Types of electronic transitions, λ_{\max} , Chromophores and Auxochromes, Bathochromic and Hypsochromic shifts, Intensity of absorption; Application of Woodward Rules for calculation of λ_{\max} for the following systems: α,β -unsaturated aldehydes, ketones, carboxylic acids and esters; Conjugated dienes: alicyclic, homoannular and heteroannular; Extended conjugated systems (aldehydes, ketones and dienes); distinction between cis and trans isomers. Application of UV Spectroscopy.

UNIT II

IR Spectroscopy: Fundamental and non-fundamental molecular vibrations; IR absorption positions of O, N and S containing functional groups; Effect of H-bonding, conjugation, resonance and ring size on IR absorptions; Fingerprint region and its significance; application in functional group analysis.

UNIT III

NMR Spectroscopy: Basic principles of Proton Magnetic Resonance, chemical shift and factors influencing it; Spin – Spin coupling and coupling constant; Anisotropic effects in alkene, alkyne, aldehydes and aromatics, Interpretation of NMR spectra of simple compounds. Applications of IR, UV and NMR for identification of simple organic molecules.

UNIT IV

Carbohydrates

Occurrence, classification and their biological importance. Monosaccharides: Constitution and absolute configuration of glucose and fructose, epimers and anomers, mutarotation, determination of ring size of glucose and fructose, Haworth projections and conformational structures; Interconversions of aldoses and ketoses; Killiani- Fischer synthesis and Ruff degradation; Disaccharides – Structure elucidation of maltose, lactose and sucrose. Polysaccharides – Elementary treatment of starch, cellulose and glycogen.

UNIT V

Dyes

Classification, Colour and constitution; Mordant and Vat Dyes; Chemistry of dyeing; Synthesis and applications of: Azo dyes – Methyl orange; Triphenyl methane dyes - Malachite green and Rosaniline ; Phthalein Dyes – Phenolphthalein; Natural dyes – structure elucidation and synthesis of Alizarin and Indigotin; Edible Dyes with examples.

Polymers

Introduction and classification including di-block, tri-block and amphiphilic polymers; Polymerisation reactions - Addition and condensation - Mechanism of cationic, anionic and free radical addition polymerization; Metallocene-based Ziegler-Natta polymerisation of alkenes; Preparation and applications of plastics – thermosetting (phenol-formaldehyde, Polyurethanes) and thermosoftening (PVC, polythene); Fabrics – natural and synthetic (acrylic, polyamido, polyester); Rubbers – natural and synthetic: Buna-S, Chloroprene and Neoprene; Vulcanization; Polymer additives; Introduction to; Biodegradable and conducting polymers with examples.

Suggested Readings

1. Kalsi, P. S. (2009). *Textbook of Organic Chemistry*. 1st Ed. New Age International (P) Ltd. Pub.
2. Morrison, R. T. & Boyd, R. N. (1992). *Organic Chemistry*. Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Billmeyer, F. W. (1984). *Textbook of Polymer Science*. John Wiley & Sons, Inc.
4. Gowariker, V. R., Viswanathan, N. V. & Sreedhar, J. (2003). *Polymer Science*. New Age International (P) Ltd. Pub.
5. Finar, I. L. (2002). *Organic Chemistry: Stereochemistry and the Chemistry of Natural Products*. Volume 2. Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
6. Clayden, J., Greeves, N., Warren, S. & Wothers, P. (2000). *Organic Chemistry*. Oxford University Press.
7. Singh, J.; Ali, S.M. & Singh, J. (2010). *Natural Product Chemistry*. Prajati Prakashan.

Course objectives

The students are able to

- Determine Field Intensity-Circular coil- Vibration magnetometer
- Co-efficient of thermal conductivity-Lee's disc method
- Refractive Index of a prism (I-I') curve-Spectrometer
- Moment of a magnet-Circular coil-Deflection Magnetometer
- Analyse the Temperature coefficient of resistance of a thermistor-Post office box
- Comparison of viscosities of two liquids
- To Study of logic gates using IC's
- To Study of NOR gate as Universal building block.
- To Study of NAND gate as Universal building block.
- Determine the Verification of Basic logic gates using discrete components.
- Determine the Cauchy's constant – Spectrometer
- AC frequency – Sonometer

Course Outcomes

- Field Intensity-Circular coil- Vibration magnetometer
- Co-efficient of thermal conductivity-Lee's disc method
- Refractive Index of a prism (I-I') curve-Spectrometer
- Moment of a magnet-Circular coil-Deflection Magnetometer
- Temperature coefficient of resistance of a thermistor-Post office box
- Comparison of viscosities of two liquids
- Study of logic gates using IC's
- Study of NOR gate as Universal building block.
- Study of NAND gate as Universal building block.
- Verification of Basic logic gates using discrete components.
- Determination of Cauchy's constant – Spectrometer
- AC frequency – Sonometer

ANY TEN EXPERIMENTS

1. Field Intensity-Circular coil- Vibration magnetometer
2. Co-efficient of thermal conductivity-Lee's disc method
3. Refractive Index of a prism (I-I') curve-Spectrometer
4. Moment of a magnet-Circular coil-Deflection Magnetometer
5. Temperature coefficient of resistance of a thermistor-Post office box
6. Comparison of viscosities of two liquids
7. Study of logic gates using IC's
8. Study of NOR gate as Universal building block.
9. Study of NAND gate as Universal building block.
10. Verification of Basic logic gates using discrete components.
11. Determination of Cauchy's constant – Spectrometer

12. AC frequency – Sonometer

References:

1. Ouseph C.C., U.J. Rao and V. Vijayendran 2007, Practical Physics and Electronics, S.Viswanathan (Printers & Publishers) Pvt. Ltd., Chennai
2. Singh S.P., 2003, Advanced Practical Physics – 1, 13th Edition, Pragathi Prakashan, Meerut
3. Singh S.P., 2000, Advanced Practical Physics – 2, 12th Edition, Pragathi Prakashan, Meerut

Course Objectives

This course enables the students to

- Perform in the conductance measurement,
- Determine of cell constant
- Determine the conductometric titrations
- Determine the kinetic aspects and rate measurements of different types of reactions.
- Determine the Acid hydrolysis of methyl acetate with hydrochloric acid.
- Determine the Saponification of ethyl acetate

Course Outcome

The Student have interpreted to

1. Measured the conductance
2. Determination of the cell constant
3. Determination of conductometric titrations
4. The kinetic aspects and rate measurements of different types of reactions.
5. Determination the Acid hydrolysis of methyl acetate with hydrochloric acid.
6. Determination of the Saponification of ethyl acetate

Conductometry:

- I. Determination of cell constant
- II. Determination of conductivity, molar conductivity, degree of dissociation and dissociation constant of a weak acid.
- III. Perform the following conductometric titrations: i. Strong acid vs. strong base ii. Weak acid vs. strong base iii. Mixture of strong acid and weak acid vs. strong base iv. Strong acid vs. weak base

Chemical Kinetics:

- IV. Study the kinetics of the following reactions.
 1. Iodide-persulphate reaction (i) Initial rate method; (ii) Integrated rate method
 2. Acid hydrolysis of methyl acetate with hydrochloric acid.
 3. Saponification of ethyl acetate.
 4. Comparison of the strengths of HCl and H₂SO₄ by studying kinetics of hydrolysis of methyl acetate.

Suggested Readings

1. Khosla, B. D., Garg, V. C. & Gulati, A. (2011). *Senior Practical Physical Chemistry*. New Delhi: R. Chand & Co.
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. (2003). *Experiments in Physical Chemistry*. 8th Ed. New York : McGraw-Hill
3. Halpern, A. M. & McBane, G. C. (2003). *Experimental Physical Chemistry*. 3rd Ed. New York: W.H. Freeman & Co.

19CHU413

ORGANIC SPECTROSCOPY - PRACTICAL

4H 2C

Instruction Hours/week:L:0 T:0 P:4Marks: Internal:40 External: 60 Total:100

End Semester Exam: 3hrs

Course objectives

The student will be able to develop and identify the

- Extraction of caffeine from tea leaves.
- Preparation of urea formaldehyde resin
- Qualitative analysis of unknown organic compounds
- Simple organic compounds by IR spectroscopy
- Simple organic compounds by NMR spectroscopy
- Preparation of methyl orange

Course outcome

The students have to categorize and demonstrate

1. About the Extraction of caffeine from tea leaves.
2. The Preparation of urea formaldehyde resin
3. The qualitative analysis of unknown organic compounds
4. Identify simple organic compounds by IR spectroscopy
5. Identify simple organic compounds by NMR spectroscopy
6. The Preparation of methyl orange

Spectroscopic methods UV, IR and NMR

1. Extraction of caffeine from tea leaves.
2. Preparation of Methyl Orange/ urea formaldehyde resin.
3. Qualitative analysis of unknown organic compounds containing monofunctional groups(carbohydrates, aryl halides, aromatic hydrocarbons, nitro compounds, amines and amides) and simple bifunctional groups, e.g. salicylic acid, cinnamic acid, nitrophenols etc.
4. Identification of simple organic compounds by IR spectroscopy and NMR spectroscopy(Spectra to be provided).

Suggested Readings

1. Vogel, A.I. (2012). *Quantitative Organic Analysis*. Part 3. Pearson.
2. Mann, F.G. & Saunders, B.C. (2009). *Practical Organic Chemistry*. Pearson Education
3. Furniss, B.S., Hannaford, A.J., Smith, P.W.G. & Tatchell, A.R. (2012). *Practical Organic Chemistry*. 5th Ed. Pearson.
4. Ahluwalia, V.K. & Aggarwal, R. (2000). *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*. University Press.
5. Ahluwalia, V.K. & Dhingra, S. (2000). *Comprehensive Practical Organic Chemistry: Qualitative Analysis*. University Press.

Course objectives

This course enables the students to

- Summarize the twelve principles of green chemistry
- To know the special emphasis of an atom economy.
- Explain the catalysis and alternate sources of energy.
- Describe the process involved in the real word cases like Surfactants for CO₂
- Synthetic azo pigments to replace toxic organic and inorganic pigments.
- Determination of environmentally safe marine antifoulant and plastic (poly lactic acid) made from corn.

Course outcome

1. Recognise the impact of green chemistry on human health and the environment.
2. Knowledge about the special emphasis of an atom economy.
3. Demonstrate the knowledge of the twelve principles of Green Chemistry which they can apply to a range of work places for a safer, less toxic and healthier environment.
4. Described the process involved in the real word cases like Surfactants for CO₂
5. Synthetic azo pigments to replace toxic organic and inorganic pigments.
6. Determination of environmentally safe marine antifoulant and plastic (poly lactic acid) made from corn.

Methodology

Blackboard teaching, Powerpoint presentation and group discussion.

UNIT I*Theory and Hand-on Experiments*

Introduction: Definitions of Green Chemistry. Brief introduction of twelve principles of Green Chemistry, with examples, special emphasis on atom economy, reducing toxicity, green solvents,

UNIT II

Green Chemistry and catalysis and alternative sources of energy, Green energy and sustainability Green energy (microwave, ultra sound and sonochemistry).

UNIT III**The following Real world Cases in Green Chemistry should be discussed:**

Surfactants for carbon dioxide – Replacing smog producing and ozone depleting solvents with CO₂ for precision cleaning and dry cleaning of garments.

UNIT IV

Designing of environmentally safe marine antifoulant. Right fit pigment: Synthetic azo pigments to replace toxic organic and inorganic pigments.

UNIT V

An efficient, green synthesis of a compostable and widely applicable plastic (polylactic acid) made from corn.

Suggested Readings

1. Anastas, P.T. & Warner, J.K. (2005). *Green Chemistry- Theory and Practical*. Oxford University Press.
2. Matlack, A.S. (2001). *Introduction to Green Chemistry*. Marcel Dekker.
3. Cann, M.C. & Connely, M.E. (2000). *Real-World cases in Green Chemistry*, American Chemical Society. Washington.

Semester-IV**19CHU404B****ANALYTICAL CLINICAL BIOCHEMISTRY 3H 3C****Instruction Hours/week: L:3 T:0 P:0 Marks: Internal: 40 External: 60 Total:100****End Semester Exam:3hrs.****Course objectives**

This course enables the student to

- Classify the basic structure of carbohydrates, and fermentation processes.
- Classification and biological importance of Proteins.
- Classification and biological importance of lipids.
- Properties, functions and biochemical functions of steroid hormones
- Know the about enzyme ,classification , mechanism and factors affectingenzyme activity.
- Identify the biochemistry of diseases.

Courseoutcome

The students have knowledge to categorize

1. The basic structure of carbohydrates.
2. Classification and biological importance of Proteins.
3. Classification and biological importance of lipids.
4. Properties, functions and biochemical functions of steroid hormones
5. Knowledge about enzyme, classification, mechanism and factors affectingenzyme activity.
6. The biochemistry of diseases.

Unit I

Carbohydrates: Biological importance of carbohydrates, Metabolism, Cellular currency ofenergy (ATP), Glycolysis, Alcoholic and Lactic acid fermentations, Krebs cycle.Isolation and characterization of polysachharides.

Unit II

Proteins: Classification, biological importance; Primary and secondary and tertiary structuresof proteins: α -helix and β -pleated sheets, Isolation, characterization, denaturation of proteins.*Enzymes:* Nomenclature, Characteristics (mention of Ribozymes), Classification; Active site,Mechanism of enzyme action, Stereospecificity of enzymes, Coenzymes and cofactors,Enzyme inhibitors, Factors affecting enzyme activity-effect of pH, temperature on enzyme activity, enzymeinhibition.

Introduction to Biocatalysis: Importance in “Green Chemistry” andChemical Industry.

Unit III

Lipids: Classification. Biological importance of triglycerides and phosphoglycerides andcholesterol; Lipid membrane, Liposomes and their biological functions and underlyingapplications.Lipoproteins.

Unit IV

Properties, functions and biochemical functions of steroid hormones. Biochemistry of peptide hormones.

Structure of DNA (Watson-Crick model) and RNA, Genetic Code, Biological roles of DNA and RNA: Replication, Transcription and Translation, Introduction to Gene therapy.

Unit V

Biochemistry of disease: A diagnostic approach by blood/ urine analysis.

Blood: Composition and functions of blood, blood coagulation. Blood collection and preservation of samples. Anaemia, Regulation, estimation and interpretation of data for blood sugar, urea, creatinine, cholesterol and bilirubin.

Urine: Collection and preservation of samples. 6. Formation of urine. Composition and estimation of constituents of normal and pathological urine.

Suggested Readings

1. Cooper, T.G. (1977). *Tool of Biochemistry*. John Wiley and Sons.
2. Keith Wilson & John Walker. (1994). *Practical Biochemistry*. Cambridge University Press.
3. Alan H Gowenlock, (2005). Varley's. *Practical Clinical Biochemistry*. CBS Publisher.
4. Thomas M. Devlin. (2009). *Textbook of Biochemistry*. Academic Internet Publishers.
5. Berg, J.M., Tymoczko, J.L. & Stryer, L. (2002). *Biochemistry*. W.H. Freeman.
6. Nelson, D. L. & Cox, M. M. (2008). *Lehninger's Principles of Biochemistry*. 7th Ed. W. H. Freeman.
7. Harwood. (1990). *Series on Analytical Chemistry*. John Wiley & Sons.

19CHU414A GREEN METHODS IN CHEMISTRY–PRACTICAL 3H 1C**Instruction Hours/week:L:0 T:0 P:3Marks: Internal:40 External: 60 Total:100****End Semester Exam: 3 hrs****Course objectives**

This course enables the student to

- Apply the principles and the practical aspects of green chemistry
- Prepare biodiesel from vegetable oil.
- Prepare phthalocyanine complex of Cu (II).
- Characterise the biodiesel.
- Mechano chemical solvent free synthesis of azomethine.
- Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper(II)

Course outcome

The students have to use

1. The basic principles and practical aspects like preparations and characterization in green approach.
2. Preparation and characterization of biodiesel from vegetable oil.
3. Characterization of biodiesel from vegetable oil.
4. Preparation of phthalocyanine complex of Cu(II).
5. Mechano chemical solvent free synthesis of azomethine.
6. Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper(II).

Practical's

1. Preparation and characterization of biodiesel from vegetable oil.
2. Preparation of phthalocyanine complex of Cu(II).
3. Mechano chemical solvent free synthesis of azomethine.
4. Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper(II).

Suggested Readings

1. Anastas, P.T. & Warner, J.K. (2005). *Green Chemistry- Theory and Practical*. Oxford University Press.
2. Matlack, A.S. (2001). *Introduction to Green Chemistry*. Marcel Dekker
3. Cann, M.C. & Connely, M.E. (2000). *Real-World cases in Green Chemistry*, American Chemical Society. Washington.
4. Ryan, M.A. & Tinnesand, M. (2002). *Introduction to Green Chemistry*. American Chemical Society. Washington.
5. Lancaster, M. (2010). *Green Chemistry: An introductory text*. 2nd Edition. RSC publishing.

Course outcome

The course enables the student to

- Identify and estimate carbohydrates.
- Identify and estimate lipids.
- Estimate the iodine number of oils
- Determine the saponification number of oils.
- Determine Cholesterol.
- Determine proteins

Course outcome

The students have to perform

1. The Identification and estimation of carbohydrates, iodine number and saponification number of oils
2. The Identification and estimation of lipids.
3. Estimation of the iodine number of oils
4. Determination the saponification number of oils.
5. Determination of Cholesterol
6. The determination of proteins

Identification and estimation of the following:

1. Carbohydrates – qualitative and quantitative.
2. Lipids – qualitative.
3. Determination of the iodine number of oil.
4. Determination of the saponification number of oil.
5. Determination of cholesterol using Liebermann- Burchard reaction.
6. Proteins – qualitative.
7. Isolation of protein.
8. Determination of protein by the Biuret reaction.
9. Determination of nucleic acids

Suggested Readings

1. Cooper, T.G. (1977). *Tool of Biochemistry*. John Wiley and Sons.
2. Keith Wilson & John Walker.(1994).*Practical Biochemistry*. Cambridge University Press.
3. Alan H Gowenlock,(2005). Varley's.*Practical Clinical Biochemistry*.CBS Publisher.
4. Thomas M. Devlin.(2009).*Textbook of Biochemistry*. Academic Internet Publishers.
5. Berg, J.M., Tymoczko, J.L. & Stryer, L.(2002).*Biochemistry*. W.H. Freeman.
6. Nelson, D. L. & Cox, M. M.(2008). *Lehninger's Principles of Biochemistry*. 7th Ed.W. H. Freeman.
7. Harwood. (1990). *Series on Analytical Chemistry*. John Wiley & Sons.

Course objectives

This course enables the student to

- Describe the principles of cheminformatics
- Explain the Representation of molecules and chemical reactions
- Predict the searching methods for chemical structures
- Predict the properties of molecules using computational methods
- QSAR studies
- Interpret the computer assisted structure elucidations.

Course outcome

The students have presented the knowledge about

1. The principles of cheminformatics
2. The Representation of molecules and chemical reactions
3. The searching methods for chemical structures
4. The prediction of the properties of molecules using computational methods
5. QSAR studies
6. The computer assisted structure elucidations

UNIT I

Introduction to Chemoinformatics: History and evolution of chemoinformatics, Use of chemoinformatics, Prospects of chemoinformatics, Molecular Modelling and Structure elucidation.

UNIT II

Representation of molecules and chemical reactions: Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.

UNIT III

Searching chemical structures: Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization.

UNIT IV

Applications: Prediction of Properties of Compounds; Linear Free Energy Relations; Quantitative Structure-Property Relations; Descriptor Analysis; Model Building; Modelling Toxicity; Structure-Spectra correlations; Prediction of NMR, IR and Mass spectra;

UNIT V

Computer Assisted Structure elucidations; Computer Assisted Synthesis Design, Introduction to drug design; Target Identification and Validation; Lead Finding and Optimization; Analysis of

HTS data; Virtual Screening; Design of Combinatorial Libraries; Ligand-Based and StructureBased Drug design; Application of Chemoinformatics in Drug Design.

Suggested Readings

1. Andrew R. Leach & Valerie, J. Gillet (2007). *An introduction to Chemoinformatics*. Springer: The Netherlands.
2. Gasteiger, J. & Engel, T. (2003). *Chemoinformatics: A text-book*. Wiley-VCH.
3. Gupta, S. P. (2011). *QSAR & Molecular Modeling*. New Delhi: Anamaya Pub.

Semester-V**19CHU501B CHEMISTRY OF COSMETICS & PERFUMES 3H 3C**

Instruction Hours/week: L:3 T:0 P:0 Marks: Internal: 40 External: 60 Total:100**End Semester Exam: 3 hrs.****Course objectives**

This skill enhancement course helps the student to

- Develop the preparation of hair dyes, hair spray and shampoos
- Develop the preparation of Hair spray
- Describe the preparation and uses of lotions,
- Describe the preparation and uses lipsticks
- Describe the preparation and uses talcum powder and Creams.
- Demonstrate the chemistry of essential oils

Course outcome

The students have formulate the knowledge about

1. The preparation of hair dyes, hair spray and shampoos
2. The preparation and uses of lotions,
3. The preparation and uses of lipsticks and
4. The preparation and uses of talcum powder
5. The preparation and uses of creams
6. The chemistry of essential oils

Unit I

A general study including preparation and uses of the following: Hair dye, hair spray, Shampoo.

Unit II

Preparation and uses of suntan lotions, face powder, lipsticks, talcum powder, nail enamel,

Unit III

Preparation and uses of creams (cold, vanishing and shaving creams), antiperspirants and artificial flavours.

Unit IV

Essential oils and their importance in cosmetic industries with reference to Eugenol, Geraniol, sandalwood oil

Unit V

Essential oils and their importance in cosmetic industries with reference to eucalyptus rose oil, 2-phenyl ethyl alcohol, Jasmone, Civetone, Muscone.

Suggested Readings

1. E. Stocchi. (1990). *Industrial Chemistry*. Vol –I. UK : Ellis Horwood Ltd.
2. P.C. Jain, M. Jain (2004). *Engineering Chemistry*. Delhi: Dhanpat Rai & Sons.
3. Sharma, B.K. & Gaur, H. (1996). *Industrial Chemistry*. Meerut : Goel Publishing House.

19CHU511A CHEMINFORMATICS- PRACTICAL 3H 1C**Instruction Hours/week: L:0 T:0 P:3 Marks: Internal:40 External: 60 Total:100****End Semester Exam: 3 hrs.****Course objectives**

The course helps the student to

- Apply the applications of cheminformatics in drug design.
- Draw the chemical structure using chemdraw software.
- Molecular docking studies were carried using Autodock software.
- Predict ADME using swissadme software
- Learn Lipinski's rule of five using swissadme software.
- 6. Predict drug likeness

Course outcome

The students know to perform the cheminformatics aspects in the drug designing process.

1. Applied the applications of cheminformatics in drug design.
2. Draw the chemical structure using chemdraw software.
3. Molecular docking studies were carried using Autodock software.
4. Prediction ADME using swissadme software
5. Learned Lipinski's rule of five using swissadme software.
6. Prediction of drug likeness

Hands-on Exercises

Application of Chemoinformatics in Drug Design

Suggested Readings

1. Andrew R. Leach & Valerie, J. Gillet. (2007). *An introduction to Chemoinformatics*. Springer: The Netherlands.
2. Gasteiger, J. & Engel, T. (2003). *Chemoinformatics: A text-book*. Wiley-VCH.
3. Gupta, S. P. (2011). *QSAR & Molecular Modeling*. New Delhi: Anamaya Pub.

Semester-V**19CHU511B CHEMISTRY OF COSMETICS & PERFUMES - PRACTICAL 3H 1C**

Instruction Hours/week: L:3 T:0 P:0 Marks: Internal: 40 External: 60 Total:100**End Semester Exam: 3 hrs.****Course objectives**

This course enables the student to

- Prepare of talcum powder.
- Prepare of shampoo.
- Prepare of enamels.
- Prepare of hair remover.
- Prepare of face cream.
- Prepare of nail polish and nail polish remover.

Course outcomes

Students have knowledge to compose about the

1. Preparation of talcum powder.
2. Preparation of shampoo.
3. Preparation of enamels.
4. Preparation of hair remover.
5. Preparation of face cream.
6. Preparation of nail polish and nail polish remover.

Preparations of cosmetics and perfumes

1. Preparation of talcum powder.
2. Preparation of shampoo.
3. Preparation of enamels.
4. Preparation of hair remover.
5. Preparation of face cream.
6. Preparation of nail polish and nail polish remover.

Suggested Readings

1. E. Stocchi. (1990). *Industrial Chemistry*, Vol –I. UK: Ellis Horwood Ltd.
2. P.C. Jain, M. Jain(2004). *Engineering Chemistry*. Delhi: Dhanpat Rai & Sons.
3. Sharma, B.K. & Gaur, H. (1996). *Industrial Chemistry*. Meerut: Goel Publishing House.

Course objectives

This course enables the student to

- Recognize the history of polymeric materials, criteria, kinetics and characterization of polymerisation.
- Criteria for polymeric material formation.
- Learn Kinetics of polymerization.
- Understand Characterisation of polymerisation.
- To know the Structure property relationships of polymer
- Justify the properties of polymers

Course outcome

The students have list the knowledge like

1. History of polymeric materials.
2. Criteria for polymeric material formation.
3. Learned Kinetics of polymerization.
4. Understood Characterisation of polymerisation.
5. Knowledge about Structure property relationships of polymer.
6. Properties of polymers.

UNIT I**Introduction and history of polymeric materials:**

Different schemes of classification of polymers, Polymer nomenclature, Molecular forces and chemical bonding in polymers, Texture of Polymers.

Functionality and its importance:

Criteria for synthetic polymer formation, classification of polymerization processes, Relationships between functionality, extent of reaction and degree of polymerization. Bifunctional systems, Poly-functional systems.

UNIT II**Kinetics of Polymerization:**

Mechanism and kinetics of step growth, radical chain growth, ionic chain (both cationic and anionic) and coordination polymerizations, Mechanism and kinetics of copolymerization, polymerization techniques.

Crystallization and crystallinity:

Determination of crystalline melting point and degree of crystallinity, Morphology of crystalline polymers, Factors affecting crystalline melting point.

UNIT III

Nature and structure of polymers-Structure Property relationships.

Determination of molecular weight of polymers (M_n , M_w , etc) by end group analysis, viscometry, light scattering and osmotic pressure methods. Molecular weight distribution and its significance. Polydispersity index.

UNIT IV

Glass transition temperature (T_g) and determination of T_g, Free volume theory, WLF equation, Factors affecting glass transition temperature (T_g).

Polymer Solution – Criteria for polymer solubility, Solubility parameter, Thermodynamics of polymer solutions, entropy, enthalpy, and free energy change of mixing of polymers solutions, Flory-Huggins theory, Lower and Upper critical solution temperatures.

UNIT V

Properties of Polymers (Physical, thermal, Flow & Mechanical Properties). Brief introduction to preparation, structure, properties and application of the following polymers: polyolefins, polystyrene and styrene copolymers, poly(vinyl chloride) and related polymers, poly(vinyl acetate) and related polymers, acrylic polymers, fluoro polymers, polyamides and related polymers. Phenol formaldehyde resins (Bakelite, Novalac), polyurethanes, silicone polymers, polydienes, Polycarbonates, Conducting Polymers, [polyacetylene, polyaniline, poly(p-phenylene sulphide), polypyrrole, polythiophene].

Suggested Readings

1. Seymour R.B., Charles E (2003). *Seymour's Polymer Chemistry: An Introduction*. Marcel Dekker, Inc.
2. G. Odian. (2004). *Principles of Polymerization*. John Wiley.
3. F.W. Billmeyer. (1972). *Text Book of Polymer Science*. John Wiley.
4. P. Ghosh. (2001). *Polymer Science & Technology*. Tata McGraw-Hill.
5. R.W. Lenz. (1968). *Organic Chemistry of Synthetic High Polymers*. John Wiley.

Course objectives

The course enables the students have to perform

- The Synthesis and modification of inorganic solids of technological importance
- Understand about the inorganic solids of technological importance
- The Synthesis and properties of nanomaterials
- The Synthesis of engineering materials used for mechanical construction
- The Synthesis and properties of composite materials
- The Synthesis and properties of speciality polymers

Course outcome

The student have identified

1. The Synthesis and modification of inorganic solids
2. Understood about inorganic solids of technological importance
3. The Synthesis and properties of nanomaterials
4. The Synthesis of engineering materials used for mechanical construction
5. The Synthesis and properties of composite materials
6. The Synthesis and properties of speciality polymers

UNIT I**Synthesis and modification of inorganic solids:**

Conventional heat and beat methods, Co-precipitation method, Sol-gel methods, Hydrothermal method, Ion-exchange and Intercalation methods.

Inorganic solids of technological importance:

Solid electrolytes – Cationic, anionic, mixed Inorganic pigments – coloured solids, white and black pigments. Molecular material and fullerenes, molecular materials & chemistry – one-dimensional metals, molecular magnets, inorganic liquid crystals.

UNIT II**Nanomaterials:**

Overview of nanostructures and nanomaterials: classification. Preparation of gold and silver metallic nanoparticles, self-assembled nanostructures-control of nanoarchitecture-one dimensional control. Carbon nanotubes and inorganic nanowires. Bio-inorganic nanomaterials, DNA and nanomaterials, natural and artificial nanomaterials, bio nano composites.

UNIT III**Introduction to engineering materials for mechanical construction:**

Composition, mechanical and fabricating characteristics and applications of various types of cast irons, plain carbon and alloy steels, copper, aluminium and their alloys like duralumin, brasses

and bronzes cutting tool materials, super alloys thermoplastics, thermosets and composite materials.

UNIT IV

Composite materials:

Introduction, limitations of conventional engineering materials, role of matrix in composites, classification, matrix materials, reinforcements, metal-matrix composites, polymer-matrix composites, fibre-reinforced composites, environmental effects on composites, applications of composites.

UNIT V

Speciality polymers:

Conducting polymers - Introduction, conduction mechanism, polyacetylene, polyparaphenylene and polypyrrole, applications of conducting polymers, Ion-exchange resins and their applications. Ceramic & Refractory: Introduction, classification, properties, raw materials, manufacturing and applications.

Suggested Readings

1. Shriver & Atkins. (2014). *Inorganic Chemistry*, Oxford University Press.
2. Peter Atkins, Tina Overton, Jonathan Rourke, Mark Weller and Fraser Armstrong. (2011-2012). 5th Edition. Oxford University Press.
3. Adam, D.M. (1974) *Inorganic Solids: An introduction to concepts in solid-state structural chemistry*. John Wiley & Sons.
4. Poole, C.P. & Owens, F.J. (2003). *Introduction to Nanotechnology*. John Wiley & Sons.
5. Rodger, G.E. (2002). *Inorganic and Solid State Chemistry*. Cengage Learning India Edition.

19CHU503	ORGANIC CHEMISTRY III:	Semester-V
	Nitrogen Containing Functional Groups, Heterocyclic chemistry and natural products	4H 4C
Instruction Hours/week:L: 4 T:0 P:0	Marks: Internal:40 External: 60 Total:100	
	End semester Exam: 3 hrs.	

Course Objectives

The students should be able

- To contrast the preparation and properties of compounds with nitrogen containing functional groups.
- Understand the preparation and properties of diazonium salts.
- Learn about polynuclear hydrocarbons,
- Know about five, six and fused membered heterocyclic compounds.
- To discuss the preparation and reactions of alkaloids
- To discuss the preparation and reactions of terpenes.

Course Outcomes

The students have summarise

1. The preparation and properties of compounds with nitrogen containing functional groups.
2. Understood the preparation and properties of diazonium salts.
3. Learned about the polynuclear hydrocarbons.
4. Knowledge about five, six and fused membered heterocyclic compounds.
5. The preparation and reactions of alkaloids
6. The preparation and reactions of terpenes.

UNIT I**Nitrogen Containing Functional Groups**

Preparation and important reactions of nitro compounds, nitriles and isonitriles.

Amines: Preparation and properties: Effect of substituent and solvent on basicity; Gabriel phthalimide synthesis, Carbylamine reaction, Mannich reaction, Hoffmann's exhaustive methylation, Hofmann-elimination reaction; Distinction between 1°, 2° and 3° amines with Hinsberg reagent and nitrous acid.

UNIT II

Diazonium Salts: Preparation and their synthetic applications.

Polynuclear Hydrocarbons

Aromaticity of polynuclear hydrocarbons, structure elucidation of naphthalene; Preparation and properties of naphthalene, phenanthrene and anthracene.

UNIT III**Heterocyclic Compounds**

Classification and nomenclature, Structure, aromaticity in 5-numbered and 6-membered rings containing one heteroatom; Synthesis, reactions and mechanism of substitution reactions of: Furan, Pyrrole (Paal-Knorr synthesis, Knorr pyrrole synthesis, Hantzsch synthesis), Thiophene, Pyridine (Hantzsch synthesis),

UNIT IV

Indole (Fischer indole synthesis and Madelung synthesis), Quinoline and isoquinoline, (Skraup synthesis, Friedlander's synthesis, Knorr quinoline synthesis, Doebner-Miller synthesis, Bischler-Napieralski reaction, Pictet-Spengler reaction, Pomeranz-Fritsch reaction)

UNIT V

Alkaloids

Natural occurrence, General structural features, Isolation and their physiological action, Hoffmann's exhaustive methylation, Emde's modification; Structure elucidation and synthesis of Nicotine. Medicinal importance of Nicotine, Hygrine, Quinine, Morphine, Cocaine, and Reserpine.

Terpenes

Occurrence, classification, isoprene rule; Elucidation of structure and synthesis of Citral.

Suggested Readings

1. Morrison, R. T. & Boyd, R. N. (1992). *Organic Chemistry*. Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Finar, I. L. (2002). *Organic Chemistry*. Volume 1. Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Finar, I. L. (2002). *Organic Chemistry: Stereochemistry and the Chemistry of Natural Products*. Volume 2. Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
4. Acheson, R.M. (1976). *Introduction to the Chemistry of Heterocyclic compounds*. John Wiley & Sons.
5. Graham Solomons, T.W. (2012). *Organic Chemistry*. John Wiley & Sons, Inc.
6. Kalsi, P. S. (2009). *Textbook of Organic Chemistry*. 1st Ed. New Age International (P) Ltd. Pub.
7. Clayden, J., Greeves, N., Warren, S. & Wothers, P. (2012). *Organic Chemistry*. Oxford University Press.
8. Singh, J.; Ali, S.M. & Singh, J. (2010). *Natural Product Chemistry*. Prajati Parakashan.

19CHU504	INORGANIC CHEMISTRY II: Metallurgy and S-Block and P-block elements	Semester-V 4H 4C
Instruction Hours/week:L: 4 T:0 P:0	Marks: Internal:40 External: 60 Total:100	End Semester Exam: 3 hrs

Course objectives

The student will recite knowledge on

- The general principles of metallurgy
- S-block elements
- Complexes of s-block elements
- Chemistry of p-block elements
- Chemistry Hydrides, oxides and oxacids
- Preparation, properties, structure and uses of some types of inorganic compounds.

Course Outcomes

It enabled the students have discuss

1. The basic principles and methods involved in the metallurgy
2. The basic properties of s-block elements and their compounds
3. The complex formation tendency of s-block elements and their structure
4. The basic properties of p-block elements and their compounds.
5. Chemistry Hydrides, oxides and oxacids
6. The preparation, properties, structure and uses of borazine, silicates, silicones, interhalogen compounds, phosphonitrilic and clathrates.

UNIT I**General Principles of Metallurgy**

Chief modes of occurrence of metals based on standard electrode potentials. Ellingham diagrams for reduction of metal oxides using carbon and carbon monoxide as reducing agent. Electrolytic Reduction, Hydrometallurgy with reference to cyanide process for silver and gold. Methods of purification of metals: Electrolytic process, Van Arkel-de Boer process and Mond's process, Zone refining.

UNIT II**Chemistry of s Block Elements:**

- (i) General characteristics: melting point, flame colour, reducing nature, diagonal relationships and anomalous behavior of first member of each group.
- (ii) Reactions of alkali and alkaline earth metals with oxygen, hydrogen, nitrogen and water.
- (iii) Common features such as ease of formation, thermal stability and solubility of the following alkali and alkaline earth metal compounds: hydrides, oxides, peroxides, superoxides, carbonates, nitrates, sulphates.

UNIT III**Complexes of s-block elements:**

- (i) Complex formation tendency of s-block elements; structure of the following complexes: crown ethers and cryptates of Group I; basic beryllium acetate, beryllium nitrate, EDTA complexes of calcium and magnesium.
- (ii) Solutions of alkali metals in liquid ammonia and their properties.

UNIT IV

Chemistry of *p* Block Elements:

Electronic configuration, atomic and ionic size, metallic/non-metallic character, melting point, ionization enthalpy, electron gain enthalpy, electronegativity, Allotropy of C, P, S; inert pair effect, diagonal relationship between B and Si and anomalous behaviour of first member of each group.

Structure, bonding and properties: acidic/basic nature, stability, ionic/covalent nature, oxidation/reduction, hydrolysis, action of heat of the following:

- Hydrides : hydrides of Group 13 (only diborane), Group 14, Group 15 (EH_3 where E = N, P, As, Sb, Bi), Group 16 and Group 17.
Oxides : oxides of phosphorus, sulphur and chlorine
Oxoacids : oxoacids of phosphorus and chlorine; peroxy acids of sulphur
Halides: halides of silicon and phosphorus

UNIT V

Preparation, properties, structure and uses of the following compounds:

- Borazine
Silicates, silicones,
Phosphonitrilic halides $\{(\text{PNCl}_2)_n \text{ where } n = 3 \text{ and } 4\}$
Interhalogen and pseudohalogen compounds
Clathrate compounds of noble gases, xenon fluorides (MO treatment of XeF_2).

Suggested Readings:

1. Lee, J.D. (2010). Concise Inorganic Chemistry. Pearson Education.
2. Douglas .B.E, Mc Daniel, D.H. & Alexander J.J. (1994). Concepts & Models of Inorganic Chemistry. 3rd Ed. N.Y. : John Wiley Sons.
3. Madan, R. L. (2015). Chemistry for Degree Students, S. Chand & Company Pvt. Ltd. Ram Nagar, New Delhi.
4. Greenwood, N.N. & Earnshaw. (2005). Chemistry of the Elements, Butterworth- Heinemann.
5. Cotton, F.A. & Wilkinson, G. (1999). Advanced Inorganic Chemistry. Wiley, VCH.
6. Miessler, G. L. & Donald, A. Tarr. (2011). Inorganic Chemistry. 5th Ed. (adapted). Pearson,
7. Shriver, D.F., Atkins P.W & Langford, C.H. (2010). Inorganic Chemistry. 5th Ed. Oxford University Press.

19CHU512A

POLYMER CHEMISTRY– PRACTICAL

Semester-V

4H 2C

Instruction Hours/week:L:0 T:0 P:4

Marks: Internal:40 External: 60

Total:100

End Semester Exam: 3 hrs.

Course objectives

This course enables the student have to apply

- Have hands on experience to prepare different types of polymers by various methods
- To do the purification of polymers
- To characterise the polymers by chemical and instrumental methods.
- To prepare isophthaloyl chloride
- Determine hydroxyl number of a polymer using colorimetric method
- Analyse the polymers

Course outcome

The students have demonstrate and perform

1. The preparation of different types of polymers by various methods
2. The purification of polymers
3. The characterization the polymers by chemical and instrumental methods.
4. Preparation of isophthaloyl chloride
5. Determination of hydroxyl number of a polymer using colorimetric method
6. Analysis of the polymers

Polymer synthesis

1. Free radical solution polymerization of styrene (St) / Methyl Methacrylate (MMA) / Methyl Acrylate (MA) / Acrylic acid (AA).
 - a. Purification of monomer
 - b. Polymerization using benzoyl peroxide (BPO) / 2,2'-azo-bis-isobutyronitrile (AIBN)
2. Preparation of nylon 66/6
 1. Interfacial polymerization, preparation of polyester from isophthaloyl chloride (IPC) and phenolphthalein
 - a. Preparation of IPC
 - b. Purification of IPC
 - c. Interfacial polymerization
3. Redox polymerization of acrylamide
4. Precipitation polymerization of acrylonitrile
5. Preparation of urea-formaldehyde resin
6. Preparations of novalac resin/resold resin.
7. Microscale Emulsion Polymerization of Poly(methylacrylate).

Polymer characterization

1. Determination of molecular weight by viscometry:
 - (a) Polyacrylamide-aq. NaNO₂ solution
 - (b) (Poly vinyl propylidene (PVP) in water
2. Determination of the viscosity-average molecular weight of poly(vinyl alcohol) (PVOH) and the fraction of —head-to-head— monomer linkages in the polymer.
3. Determination of molecular weight by end group analysis: Polyethylene glycol (PEG) (OH group).

4. Testing of mechanical properties of polymers.
5. Determination of hydroxyl number of a polymer using colorimetric method.

Polymer analysis

1. Estimation of the amount of HCHO in the given solution by sodium sulphite method
2. Instrumental Techniques
3. IR studies of polymers
4. DSC analysis of polymers
5. Preparation of polyacrylamide and its electrophoresis
*at least 7 experiments to be carried out.

Suggested Readings

1. Malcolm P. Stevens(1999). *Polymer Chemistry: An Introduction*.3rd Ed. Oxford University Press.
2. Harry R. Allcock, Frederick W. Lampe and James E. Mark, (2003). *Contemporary Polymer Chemistry*.3rd ed. Prentice-Hall
3. Fred W. Billmeyer, (1984). *Textbook of Polymer Science*.3rd ed. Wiley-Interscience
4. Joel R. Fried, (2003). *Polymer Science and Technology*.2nd ed. Prentice-Hall.
5. Petr Munk & Tejraj M. Aminabhavi, (2002). *Introduction to Macromolecular Science*. 2nd ed. John Wiley & Sons
6. L. H. Sperling,.(2005). *Introduction to Physical Polymer Science*.4th ed. John Wiley & Sons.
7. Malcolm P. Stevens, (2005). *Polymer Chemistry: An Introduction*. 3rd ed. Oxford University Press.
8. Charles E. Carraher,.(2013). *Seymour/ Carraher's Polymer Chemistry*. 9th ed. Jr.

19CHU512BNOVEL INORGANIC SOLIDS-PRACTICAL4H 2C**Instruction Hours/week: L:0 T:0 P:04 Marks: Internal: 40 External: 60 Total:100****End Semester Exam: 3 hrs.****Course objectives**

The course helps the student to

- Explain the ion exchange method
- Explain the cation exchange method
- coprecipitation methods of novel inorganic solids
- Discuss the method for the preparation of nanoparticles
- Nano partical preparation using green method
- Prepare the hydrogel by coprecipitation method

Course outcome

The students have demonstrated

1. The cation exchange method
2. The ion exchange method
3. coprecipitation methods of novel inorganic solids
4. The method for the preparation of nanoparticles
5. Nano partical preparation using green method
6. Preparation of the hydrogel by coprecipitation method

Preparation of nano particles, coprecipitation method

1. Determination of cation exchange method
2. Determination of total difference of solids.
3. Synthesis of hydrogel by co-precipitation method.
4. Synthesis of metal nanoparticles.

Suggested Reading:

1. Fahlman, B.D. (2004). *Materials Chemistry*, Springer.

**19CHU513 NITROGEN CONTAINING FUNCTIONAL GROUPS, 4H 2C
HETEROCYCLIC CHEMISTRY AND NATURAL PRODUCTS - PRACTICAL****Instruction Hours/week: L: 0 T: 0 P: 4 Marks: Internal: 40 External: 60 Total: 100****End semester exam: 3 hrs.****Course Objective**

This course enables the student to

- Identify the presence of nitro
- Identify the presence of amine
- Identify the presence of amide groups
- Identify functional groups like alcohols.
- Identify functional groups of carboxylic acids.
- Identify the functional groups like phenols, carbonyl compounds and esters

Course Outcome

The students have analysed the

1. Functional group tests for nitrogen containing organic compounds
 2. Identification of nitro group
 3. Identification of amine group
 4. Identification of amide
 5. Tests used in the Identification of functional groups like alcohols, carboxylic acids
 6. Identification of phenols, carbonyl compounds and esters
-
1. Functional group test of nitro, amine and amide groups.
 2. Qualitative analysis of unknown organic compounds containing simple functional groups (alcohols, carboxylic acids, phenols, carbonyl compounds and esters)

Suggested Readings

1. Mann, F.G. & Saunders, B.C. (2009). *Practical Organic Chemistry*. Pearson Education
2. Furniss, B.S., Hannaford, A.J., Smith, P.W.G. & Tatchell, A.R. (2012). *Practical Organic Chemistry*. 5th Ed. Pearson.
3. Ahluwalia, V.K. & Aggarwal, R. (2000). *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*. University Press
4. Ahluwalia, V.K. & Dhingra, S. (2000). *Comprehensive Practical Organic Chemistry: Qualitative Analysis*. University Press.

19CHU514	S-BLOCK AND P-BLOCK ELEMENTS – PRACTICAL	Semester-V
		4H 2C
Instruction Hours/week:L: 0 T:0 P:4	Marks: Internal:40	External: 60 Total:100
		End Semester Exam: 3 hrs

Course Objectives

The students have to analyse

- The estimate the metal ions by iodimetric titrations
- The estimate the metal ions by complexometric titrations using EDTA
- The carryout the preparations of inorganic metal complexes.
- Prepare cuprous chloride
- Prepare Manganese (III) phosphate
- Prepare potash alum and chrome alum.

Course Outcomes

The students have analyse

1. The iodometric titration methods.
2. The complexometric titration methods
2. The preparation the s and p-block metal complexes.
4. Preparation of cuprous chloride
5. Preparation of Manganese (III) phosphate
6. Preparation of potash alum and chrome alum.

(A) Iodo / Iodimetric Titrations

- (i) Estimation of Cu(II) and $K_2Cr_2O_7$ using sodium thiosulphate solution (Iodometrically).
- (ii) Estimation of Potassiumdichromate using sodiumthiosulphate solution iodimetrically

(B) Complexometric titrations using disodium salt of EDTA

- (i) Estimation of Mg^{2+} , Zn^{2+}
- (ii) Estimation of Ca^{2+} by substitution method

(C) Inorganic preparations

- (i) Cuprous Chloride, Cu_2Cl_2
- (ii) Manganese (III) phosphate, $MnPO_4 \cdot H_2O$
- (iii) Aluminium potassium sulphate $KAl(SO_4)_2 \cdot 12H_2O$ (Potash alum) or Chrome alum.

Suggested Readings

1. Vogel, A.I. (1978). A Textbook of Quantitative Inorganic Analysis, ELBS.
2. Marr, G. and Rockett, R.W. (1972). Practical Inorganic Chemistry, Van Nostrand Reinhold.
3. Deepak Pant.P. (2010). Inorganic Chemistry Practical, BookRix.

Semester-VI

19CHU601A

BASIC ANALYTICAL CHEMISTRY

3H 3C

Instruction Hours/week: L:3 T:0 P:0 Marks: Internal:40 External: 60 Total:100

End Semester Exam: 3 hrs.

Course objectives

The course enables the students have to interpret

- The interdisciplinary nature of analytical chemistry
- The various methods involved in the analysis of soil ,
- Analyse water
- Analys food products
- Concepts of pH
- The various methods involved in the analysis of cosmetics

Course outcome

The course enables the students have to interpreted

1. The interdisciplinary nature of analytical chemistry
2. The various methods involved in the analysis of soil ,
3. Analysis water
4. Analysis of food products
5. Concepts of pH
6. The various methods involved in the analysis of cosmetics

UNIT I

Introduction: Introduction to Analytical Chemistry and its interdisciplinary nature. Concept of sampling. Importance of accuracy, precision and sources of error in analytical measurements. Presentation of experimental data and results, from the point of view of significant figures.

UNIT II

Analysis of soil: Composition of soil, Concept of pH and pH measurement, Complexometric titrations, Chelation, Chelating agents, use of indicators

- a. Determination of pH of soil samples.
- b. Estimation of Calcium and Magnesium ions as Calcium carbonate by complexometric titration.

UNIT III

Analysis of water: Definition of pure water, sources responsible for contaminating water, water sampling methods, water purification methods.

- a. Determination of pH, acidity and alkalinity of a water sample.
- b. Determination of dissolved oxygen (DO) of a water sample.

UNIT IV

Analysis of food products: Nutritional value of foods, idea about food processing and food preservations and adulteration.

- a. Identification of adulterants in some common food items like coffee powder, asafoetida, chilli powder, turmeric powder, coriander powder and pulses, etc.
- b. Analysis of preservatives and colouring matter.

Chromatography: Definition, general introduction on principles of chromatography, paper chromatography, TLC etc.

- a. Paper chromatographic separation of mixture of metal ion (Fe^{3+} and Al^{3+}).
- b. To compare paint samples by TLC method.

Ion-exchange: Column, ion-exchange chromatography etc. Determination of ion exchange capacity of anion / cation exchange resin (using batch procedure if use of column is not feasible).

UNIT V

Analysis of cosmetics: Major and minor constituents and their function

- a. Analysis of deodorants and antiperspirants, Al, Zn, boric acid, chloride, sulphate.
- b. Determination of constituents of talcum powder: Magnesium oxide, Calcium oxide, Zinc oxide and Calcium carbonate by complexometric titration.

Suggested Reading

1. Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. (1988). *Instrumental Methods of Analysis*. 7th Ed. Belmont, California, USA : Wadsworth Publishing Co. Ltd.
2. Skoog, D.A. Holler F.J. & Nieman, T.A. (1998). *Principles of Instrumental Analysis*, Cengage Learning India Ed.
3. Skoog, D.A.; West, D.M. & Holler, F.J. (1992). *Fundamentals of Analytical Chemistry* 6th Ed. Fort Worth : Saunders College Publishing.
4. Harris, D. C. (2006). *Quantitative Chemical Analysis*. W. H. Freeman and Company Ltd., Dean, J. A. (1992). *Analytical Chemistry Notebook*. McGraw Hill.
5. Day, R. A. & Underwood, A. L. (1991). *Quantitative Analysis*. Prentice Hall of India.
6. Freifelder, D. (1982). *Physical Biochemistry*. 2nd Ed. N.Y. USA: W.H. Freeman and Co.
7. Cooper, T.G. (1977). *The Tools of Biochemistry*. 16. N.Y. USA: John Wiley and Sons.
8. Robinson, J.W. (1995). *Undergraduate Instrumental Analysis*. 5th Ed. New Delhi: Marcel Dekker Inc.,

19CHU601B PESTICIDE CHEMISTRY 3H 3C**Instruction Hours/week: L:3 T:0 P:0 Marks: Internal: 40 External: 60 Total:100****End Semester Exam: 3 hrs.****Course objectives**

The course enables the students to design

- The synthesis and manufacture of many natural fertilizers
- The synthesis and manufacture of many synthetic fertilizers
- The synthesis and manufacture of organochlorines
- The synthesis and manufacture organophosphorous compounds
- The synthesis and manufacture of quinine pesticides
- The synthesis and manufacture of anilides

Course outcomes

The students have designed

1. The synthesis and manufacture of many natural fertilizers
2. The synthesis and manufacture of many synthetic fertilizers
3. The synthesis and manufacture of organochlorines
4. The synthesis and manufacture organophosphorous compounds
5. The synthesis and manufacture of quinine pesticides
6. The synthesis and manufacture of anilides

Unit I

General introduction to pesticides (natural and synthetic), benefits and adverse effects.

Unit II

Changing concepts of pesticides, structure activity relationship.

Unit III

Synthesis and technical manufacture and uses of representative pesticides in the following classes: Organochlorines (DDT, Gammexene,)

Unit IV

Synthesis and technical manufacture and uses of Organophosphates (Malathion, Parathion); Carbamates (Carbofuran and carbaryl)

Unit V

Synthesis and technical manufacture and uses of Quinones (Chloranil), Anilides (Alachlor and Butachlor).

Suggested Reading

1. Cremllyn, R. (1978). *Pesticides. Preparation and Modes of Action*. New York: John Wiley & So

Course objectives

The course enables the students have to interpret

- Estimation of macro nutrients
- The various methods involved in the analysis of soil ,
- Analyse of water
- Analyse food products
- Spectrophotometric Identification and Determination of Caffeine and Benzoic Acid in SoftDrink
- Spectrophotometric determination of Iron in Vitamin

Course outcome

The course enables the students have to interpreted

1. Estimation of macro nutrients
2. The various methods involved in the analysis of soil
3. Analysis water
4. Analysis of food products
5. The various methods involved in the analysis of cosmetics
6. Spectrophotometric Identification and Determination of Caffeine and Benzoic Acid in SoftDrink
7. Spectrophotometric determination of Iron in Vitamin

Applications (Any one):

- a. To study the use of phenolphthalein in traps cases.
- b. To analyze arson accelerants.
- c. To carry out analysis of gasoline.

Instrumental demonstrations:

- a. Estimation of macro nutrients: Potassium, Calcium, Magnesium in soil samples by flamephotometry.
- b. Spectrophotometric determination of Iron in Vitamin / Dietary Tablets.
- c. Spectrophotometric Identification and Determination of Caffeine and Benzoic Acid in Soft Drink.

Suggested Reading

1. Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. (1988). *Instrumental Methods of Analysis*. 7th Ed. Belmont, California, USA : Wadsworth Publishing Co. Ltd.
2. Skoog, D.A. Holler F.J. & Nieman, T.A.(1998). *Principles of Instrumental Analysis*, Cengage Learning India Ed.

3. Skoog, D.A.; West, D.M. & Holler, F.J.(1992).*Fundamentals of Analytical Chemistry* 6th Ed.Fort Worth :Saunders College Publishing.
4. Harris, D. C. (2006). *Quantitative Chemical Analysis*. W. H. Freeman and Company Ltd.,
5. Dean, J. A. (1992). *Analytical Chemistry Notebook*. McGraw Hill.
6. Day, R. A. & Underwood, A. L. (1991). *Quantitative Analysis*. Prentice Hall of India.
7. Freifelder, D. (1982).*Physical Biochemistry*.2nd Ed.N.Y. USA: W.H. Freeman and Co.
8. Cooper, T.G. (1977).*The Tools of Biochemistry*.16.N.Y. USA: John Wiley and Sons.
9. Robinson, J.W.(1995). *Undergraduate Instrumental Analysis*.5th Ed.NewDelhi:Marcel Dekker Inc.,

Semester-VI

19CHU611B PESTICIDE CHEMISTRY-PRACTICAL3H 1C**Instruction Hours/week: L:3 T:0 P:0Marks: Internal: 40 External: 60 Total:100****End Semester Exam: 3 hrs.****Course objectives**

The lab course enables the student to solve

- the calculation of acidity in given sample of pesticide formulation
- the calculation of alkalinity in given sample of pesticide formulation
- the synthesis of simple organophosphates,
- the synthesis of phosphonates
- the synthesis of thiophosphates
- Alayse organophosphates, phosphonates and thiophosphates

Course outcomes

The students have solved

1. the calculation of acidity in given sample of pesticide formulation
2. the calculation of alkalinity in given sample of pesticide formulation
3. the synthesis of simple organophosphates
4. the synthesis of phosphonates
5. the synthesis of thiophosphates
6. Alaysis of organophosphates, phosphonates and thiophosphates

Practicals

1. To calculate acidity/alkalinity in given sample of pesticide formulations.
2. Preparation of simple organophosphates, phosphonates and thiophosphates

Suggested Reading:

1. Cremlyn, R.(1978).*Pesticides. Preparation and Modes of Action*. NewYork: John Wiley & Sons.

Course Objectives

This course enables the student to discuss

- The Theoretical Principles in Qualitative Analysis to identify the cations and anions
- The classification of organometallic compounds based on bond type
- The few important metal complexes of commercial importance
- About 18 electron rule
- The catalytic property of organometallic compounds.
- The Metal ions present in biological systems

Course Outcome

The student have discussed

1. The Theoretical Principles in Qualitative Analysis to identify the cations and anions
2. The classification of organometallic compounds based on bond type
3. Few important metal complexes of commercial importance
4. About 18 electron rule
5. The catalytic property of organometallic compounds.
6. The Metal ions present in biological systems

UNIT I**Theoretical Principles in Qualitative Analysis (H₂S Scheme)**

Basic principles involved in analysis of cations and anions. Solubility products, common ion effect. Principles involved in separation of cations into groups and choice of group reagents. Interfering anions (fluoride, borate, oxalate and phosphate) and need to remove them after Group II.

UNIT II**Organometallic Compounds**

Definition and classification of organometallic compounds on the basis of bond type. Concept of hapticity of organic ligands. Metal carbonyls: 18 electron rule, electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series. General methods of preparation (direct combination, reductive carbonylation, thermal and photochemical decomposition) of mono and binuclear carbonyls of 3d series. Structures of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni using VBT. π -acceptor behaviour of CO (MO diagram of CO to be discussed), synergic effect and use of IR data to explain extent of back bonding.

UNIT III

Zeise's salt: Preparation and structure, evidences of synergic effect and comparison of synergic effect with that in carbonyls. Metal Alkyls: Important structural features of methyl lithium (tetramer) and trialkyl aluminium (dimer), concept of multicentre bonding in these compounds. Ferrocene: Preparation and reactions (acetylation, alkylation, metallation, Mannich Condensation). Structure and aromaticity. Comparison of aromaticity and reactivity with that of benzene.

UNIT IV

Catalysis by Organometallic Compounds

Study of the following industrial processes and their mechanism:

1. Alkene hydrogenation (Wilkinson's Catalyst)
2. Synthetic gasoline (Fischer Tropsch reaction)
3. Polymerisation of ethene using Ziegler-Natta catalyst

UNIT V

Metal ions present in biological systems, classification of elements according to their action in biological system. Geochemical effect on the distribution of metals. Sodium / K-pump, carbonic anhydrase and carboxypeptidase. Excess and deficiency of some trace metals. Toxicity of metal ions (Hg, Pb, Cd and As), reasons for toxicity, Use of chelating agents in medicine, Cisplatin as an anti-cancer drug. Iron and its application in bio-systems, Haemoglobin, Myoglobin; Storage and transfer of iron.

Suggested Readings

1. Cotton, F.A., Wilkinson, G., & Gaus, P.L.(1993). *Basic Inorganic Chemistry*. 3rd Ed. Wiley India.
2. Huheey, J. E., Keiter, E.A. & Keiter, R.L. (2006). *Inorganic Chemistry: Principles of Structure and Reactivity*. 4th Ed. Harper Collins. Pearson.
3. Sharpe, A.G. (2005). *Inorganic Chemistry*, 4th Indian Reprint. Pearson Education.
4. Douglas, B. E.; McDaniel, D.H. & Alexander, J.J.(1994). *Concepts and Models in Inorganic Chemistry*. 3rd Ed. NY: John Wiley and Sons.
5. Greenwood, N.N. & Earnshaw, A. (1997). *Chemistry of the Elements*. 2nd Ed, Elsevier, (Ziegler Natta Catalyst and Equilibria in Grignard Solution).
6. Lee, J.D. (2008). *Concise Inorganic Chemistry*. 5th Ed. John Wiley and sons.
7. Powell, P. (1988). *Principles of Organometallic Chemistry*, Chapman and Hall.
8. Shriver, D.D., Atkins, P. and Langford, C.H. (1994). *Inorganic Chemistry*. 2nd Ed. Oxford University Press.
9. Miessler, G. L. & Tarr, Donald A. (2010). *Inorganic Chemistr*. 4th Ed. Pearson.
10. Crabtree, Robert H. (2000). *The Organometallic Chemistry of the Transition Metals*. NY: John Wiley New York.
11. Spessard, Gary O., & Miessler, Gary L. (1996). *Organometallic Chemistry*. Upper Saddle River, NJ: Prentice-Hall.

Semester-I

4H 4C

19CHU603

PHYSICAL CHEMISTRY I: States of matter and ionic equilibrium**Instruction Hours/week:L: 4 T:0 P:0 Marks: Internal:40 External: 60 Total:100****End Semester Exam: 3 hrs****Course objectives**

Enable the students to identify

- The Kinetic molecular model of a gas and about the molecular velocities
- The behaviour of real gases
- The structure of the liquid state and its properties like surface tension and viscosity.
- The solid state, symmetries present and different types of crystals.
- The theory of ionic equilibria, ionisation of electrolytes and salt hydrolysis.
- The buffer solutions and acid-base titrations.

Course outcomes

Students are able to

1. Explain the origin of K_{eq} and its relation to fugacity and activity and apply these concepts to ideal and real solutions of electrolytes and non-electrolytes and to colligative properties.
2. Apply the principles of electrochemistry to conductance, voltaic, and electrolytic systems.
3. Provide a physical basis for Debye-Huckel theory.
4. List the methods for arriving at a plausible mechanism and/or rate law based on kinetic information.
5. Manipulate the gas laws to describe real and ideal gas behavior.
6. Apply the steady-state hypothesis to obtain rate equations. Explain the basic principles of photochemical and radiation-chemical reactions.

UNIT I

Gaseous state: Kinetic molecular model of a gas: postulates and derivation of the kinetic gas equation; collision frequency; collision diameter; mean free path and viscosity of gases, including their temperature and pressure dependence, relation between mean free path and coefficient of viscosity, calculation of ζ from η ; variation of viscosity with temperature and pressure. Maxwell distribution and its use in evaluating molecular velocities (average, root mean square and most probable) and average kinetic energy, law of equipartition of energy, degrees of freedom and molecular basis of heat capacities.

UNIT II

Behaviour of real gases: Deviations from ideal gas behaviour, compressibility factor, Z , and its variation with pressure and temperature for different gases. Causes of deviation from ideal behaviour. Van der Waals equation of state, its derivation and application in explaining real gas behaviour, calculation of Boyle temperature. Isotherms of real gases and their comparison with

Van der Waals isotherms, continuity of states, critical state, relation between critical constants and Van der Waals constants, law of corresponding states.

Liquid state: Qualitative treatment of the structure of the liquid state; physical properties of liquids, vapour pressure, surface tension coefficient of viscosity, and their determination. Effect of addition of various solutes on surface tension and viscosity. Explanation of cleansing action of detergents. Temperature variation of viscosity of liquids and comparison with that of gases.

UNIT III

Solid state: Nature of the solid state, law of constancy of interfacial angles, law of rational indices, Miller indices, elementary ideas of symmetry, symmetry elements and symmetry operations, qualitative idea of point and space groups, seven crystal systems and fourteen Bravais lattices; X-ray diffraction, Bragg's law, a simple account of rotating crystal method and powder pattern method. Analysis of powder diffraction patterns of NaCl, CsCl and KCl.

UNIT IV

Ionic equilibria: Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect; Ostwald dilution law, dissociation constants of mono and diprotic acids. Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts.

UNIT V

Buffer solutions; derivation of Henderson equation and its applications. Solubility and solubility product of sparingly soluble salts – applications of solubility product principle. Qualitative treatment of acid – base titration curves (calculation of pH at various stages). Theory of acid–base indicators; selection of indicators and their limitations.

Suggested Readings:

1. Atkins, P. W. & Paula, J. de Atkin's. (2006). Physical Chemistry Ed. Oxford University Press.
2. Ball D. W. (2007). Physical Chemistry. India : Thomson Press.
3. Madan, R. L. (2015). Chemistry for Degree Students, S. Chand & Company Pvt. Ltd. Ram Nagar, New Delhi.
4. Castellan, G. W. (2004). Physical Chemistry. 4th Ed. Narosa.
5. Mortimer, R. G. (2009). Physical Chemistry. 3rd Ed. NOIDA, UP : Elsevier.

Course Objectives

This lab course enables the student to

- Identify the anions and the cations in a mixture by Qualitative semimicro analysis
- Understand the chemistry of different reactions
- Identify the interfering anion
- Outline the principles behind the spot tests
- chromatographic separations
- Paper chromatographic separation of nickel and cobalt, copper and cadmium

Course Outcome

The students have

1. Identified the anions and the cations in a mixture by Qualitative semi micro analysis
2. Understood the chemistry of different reactions.
3. Identified the interfering anion
4. Define the principles behind the spot tests and
5. Define the Principles of chromatographic separations
6. Paper chromatographic separation of nickel and cobalt, copper and cadmium

Qualitative semimicro analysis of mixtures containing 3 anions and 3 cations. Emphasis should be given to the understanding of the chemistry of different reactions. The following radicals are suggested:

CO_3^{2-} , NO_2^- , S^{2-} , SO_3^{2-} , $\text{S}_2\text{O}_3^{2-}$, CH_3COO^- , F^- , Cl^- , Br^- , I^- , NO_3^- , BO_3^{3-} , $\text{C}_2\text{O}_4^{2-}$, PO_4^{3-} , NH_4^+ , K^+ , Pb^{2+} , Cu^{2+} , Cd^{2+} , Bi^{3+} , Sn^{2+} , Sb^{3+} , Fe^{3+} , Al^{3+} , Cr^{3+} , Zn^{2+} , Mn^{2+} , Co^{2+} , Ni^{2+} , Ba^{2+} , Sr^{2+} , Ca^{2+} , Mg^{2+}

Mixtures should preferably contain one interfering anion, **or** insoluble component (BaSO_4 , SrSO_4 , PbSO_4 , CaF_2 or Al_2O_3) **or** combination of anions e.g. CO_3^{2-} and SO_3^{2-} , NO_2^- and NO_3^- ,

Cl^- and Br^- , Cl^- and I^- , Br^- and I^- , NO_3^- and Br^- , NO_3^- and I^-

Spot tests should be done whenever possible.

Principles involved in chromatographic separations. Paper chromatographic separation of following metal ions:

- i. Ni (II) and Co (II)
- ii. Cu(II) and Cd(II)

Suggested Reading

1. Svehla, G. (1996) Vogel's *Qualitative Inorganic Analysis*, Longman, New York.

Semester-VI**19CHU613****STATES OF MATTER AND****2H 1C****IONIC EQUILIBRIUM - PRACTICAL****Instruction Hours/week:L: 0 T:0 P:2Marks: Internal:40 External: 60 Total:100****End Semester Exam: 3 hrs****Course Objectives**

The students develop the skills to categorize

- Surface tension of a liquid
- Study the variation of surface tension with different concentration of detergent solutions.
- Viscosity of a liquid
- Prepare a buffer solution and to measure its pH.
- Monitor the pH of a solution during the course of a titration.
- Indexing of a given powder diffraction pattern of a cubic crystalline system.

Course Outcomes

The students develops the practical skill have categorized the

1. Determination of surface tension of a liquid
2. Determination the viscosity of a liquid
3. Prepare a buffer solution and to measure the pH of a solution
4. Monitor the pH of a solution during the course of a titration.
5. The lab will also provide hands-on opportunities to develop and apply this knowledge
6. Indexing of a given powder diffraction pattern of a cubic crystalline system.

1. Surface tension measurements

- a. Determination of the surface tension of a liquid.
- b. Study the variation of surface tension with different concentration of detergent solutions.

2. Viscosity measurement.

- a. Determination of co-efficient of viscosity of an unknown aqueous solution.
- b. Study the variation of co-efficient of viscosity with different concentration of Poly VinylAlcohol (PVA) and determine molar of PVA.
- b. Study the variation of viscosity with different concentration of sugar solutions.

3. Solid State:

- a. Indexing of a given powder diffraction pattern of a cubic crystalline system.

4. pH metry:

- a. Study the effect of addition of HCl/NaOH on pH to the solutions of acetic acid, sodium acetate and their mixtures.
- b. Preparation of buffer solutions of different pH values (i). Sodium acetate-acetic acid (ii).Ammonium chloride-ammonium hydroxide
- c. pH metric titration of (i) strong acid with strong base, (ii) weak acid with strong base. Determination of dissociation constant of a weak acid.

Suggested Readings:

1. Khosla, B. D., Garg, V. C. & Gulati, A.(2011).Senior Practical Physical Chemistry. New Delhi :R. Chand &Co.
 2. Garland, C. W., Nibler, J. W. & Shoemaker, D. P. (2003). Experiments in Physical Chemistry. 8th Ed.New York : McGraw-Hill.
 3. Halpern, A. M. & McBane, G. C.(2003).Experimental Physical Chemistry. 3rd Ed. New York : W.H. Freeman & Co.
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Course objectives

The course enables the students to summarize

- The introductory concepts of molecular modelling
- The force fields involved with different types of interactions
- The Energy Minimization and Computer Simulation
- The Molecular Dynamics & Monte Carlo Simulation
- The Structure Prediction and Drug Design
- QSAR studies

Course outcomes

The students are contrast

1. The introductory concepts of molecular modelling
2. The force fields involved with different types of interactions
3. About the Energy Minimization and Computer Simulation
4. About the Molecular Dynamics & Monte Carlo Simulation
5. About the Structure Prediction and Drug Design
6. QSAR studies

UNIT I**Introduction to Molecular Modelling:**

Introduction. Useful Concepts in Molecular Modelling: Coordinate Systems. Potential Energy Surfaces. Molecular Graphics. Surfaces. Computer Hardware and Software. The Molecular Modelling Literature.

UNIT II**Force Fields:**

Fields. Bond Stretching. Angle Bending. Introduction to nonbonded interactions. Electrostatic interactions. van der Waals Interactions. Hydrogen bonding in Molecular Mechanics. Force Field Models for the Simulation of Liquid Water.

UNIT III**Energy Minimization and Computer Simulation:**

Minimization and related methods for exploring the energy surface. Non-derivative method, First and second order minimization methods. Computer simulation methods. Simple thermodynamic properties and Phase Space. Boundaries. Analyzing the results of a simulation and estimating Errors.

UNIT IV**Molecular Dynamics & Monte Carlo Simulation:**

Molecular Dynamics Simulation Methods. Molecular Dynamics using simple models. Molecular Dynamics with continuous potentials. Molecular Dynamics at constant temperature and pressure. Metropolis method. Monte Carlo simulation of molecules. Models used in Monte Carlo simulations of polymers.

UNIT V

Structure Prediction and Drug Design:

Structure prediction - Introduction to comparative Modeling. Sequence alignment. Constructing and evaluating a comparative model. Predicting protein structures by 'Threading', Molecular docking. Structure based de novo ligand design, Drug Discovery – Chemoinformatics – QSAR.

Suggested Readings

1. Leach, A.R. (2001). *Molecular Modelling Principles and Application*, Longman.
2. Haile, J.M. (1997). *Molecular Dynamics Simulation Elementary Methods*, John Wiley and Sons.
3. Gupta, S.P. (2008). *QSAR and Molecular Modeling*. Springer. Anamaya Publishers.

19CHU614 MOLECULAR MODELLING AND DRUG DESIGN-PRACTICAL 4H 2C**Instruction Hours/week: L:0 T:0 P:4 Marks: Internal:40 External: 60 Total:100****End Semester Exam: 3 hrs.****Course objectives**

The lab course enables the students to analyse

- Qualitative and quantitative calculations involved in the molecular modelling and its usefulness in drug design
- Compare the optimized C-C bond lengths in ethane, ethene, ethyne and benzene. Visualize the molecular orbitals of the ethane σ bonds and ethene, ethyne, benzene and pyridine π bonds.
- Perform a conformational analysis of butane. (b)
- Determine the enthalpy of isomerization of *cis* and *trans*-2-butene.
- Relate the charge on the hydrogen atom in hydrogen halides with their acid character.
- Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine.
- Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol.

Course outcomes

The students have analysed

1. The Qualitative and quantitative calculations involved in the molecular modelling and its usefulness in drug design
 2. Comparison of the optimized C-C bond lengths in ethane, ethene, ethyne and benzene. Visualize the molecular orbitals of the ethane σ bonds and ethene, ethyne, benzene and pyridine π bonds.
 3. Performed a conformational analysis of butane.
 4. Determination of the enthalpy of isomerization of *cis* and *trans*-2-butene.
 5. Relate the charge on the hydrogen atom in hydrogen halides with their acid character.
 6. Comparison of the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol.
 7. Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol.
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- i. Compare the optimized C-C bond lengths in ethane, ethene, ethyne and benzene. Visualize the molecular orbitals of the ethane σ bonds and ethene, ethyne, benzene and pyridine π bonds.
 - ii. (a) Perform a conformational analysis of butane. (b) Determine the enthalpy of isomerization of *cis* and *trans*-2-butene.
 - iii. Visualize the electron density and electrostatic potential maps for LiH, HF, N₂, NO and CO and comment. Relate to the dipole moments. Animate the vibrations of these molecules.

- iv. (a) Relate the charge on the hydrogen atom in hydrogen halides with their acid character. (b) Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine.
- v. (a) Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol. Note the dipole moment of each molecule. (b) Show how the shapes affect the trend in boiling points: (118 °C, 100 °C, 108 °C, 82 °C, respectively).
- vi. Build and minimize organic compounds of your choice containing the following functional groups. Note the dipole moment of each compound: (a) alkyl halide (b) aldehyde (c) ketone (d) amine (e) ether (f) nitrile (g) thiol (h) carboxylic acid (i) ester (j) amide.
- vii. (a) Determine the heat of hydration of ethylene. (b) Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.
- viii. Arrange 1-hexene, 2-methyl-2-pentene, (*E*)-3-methyl-2-pentene, (*Z*)-3-methyl-2-pentene, and 2,3-dimethyl-2-butene in order of increasing stability.
- ix. (a) Compare the optimized bond angles H₂O, H₂S, H₂Se. (b) Compare the HAH bond angles for the second row dihydrides and compare with the results from qualitative MO theory.

Note: Software: ChemSketch, ArgusLab (www.planaria-software.com), TINKER 6.2 (dasher.wustl.edu/ffe), WebLab Viewer, Hyperchem, or any similar software

Suggested Readings

1. Leach, A.R. (2001). *Molecular Modelling Principles and Application*. Longman.
2. Haile, J.M. (1997). *Molecular Dynamics Simulation Elementary Methods*, John Wiley and Sons.
3. Gupta, S.P. (2008). *QSAR and Molecular Modeling*. Springer - Anamaya Publishers.

19CHU691**PROJECT WORK****Semester-VI****8H 6C**

Instruction Hours/week: L:0 T:0 P:8Marks: Internal: 40 External: 60 Total:100