



**Program**

**M Sc - Chemistry**

**Faculty of Science**

**(Revised with effect from 2018-19 AY onwards)**

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## Programme Outcomes

1. **Scientific Knowledge and Pursuit:** Gain and apply knowledge of basic scientific and mathematical fundamentals, to develop deeper understanding Nature and apply it to develop new theories and models.
2. **Theoretical Methods & Problem Analysis:** Develop analytical skills to analyse complex phenomena using first principles enabling one to identify underlying structure.
3. **Experimental Skills and Development of solutions:** Use of research-based knowledge and research methods including design of physical/computational experiments, Design of solutions for complex chemistry/physics/ mathematics problems and evolve procedures appropriate to a given problem.
4. **Computational, Numerical and Data Analysis:** Numerical analysis and simulation modelling and interpretation of data, and synthesis of the information to provide valid conclusions.
5. **Modern Analytical Tool Usage:** Select, and apply appropriate techniques, resources, and modern analytical tools.
6. **Scientific Communication:** Communicate orally and in writing on complex scientific activities with peers, educators, science community, and with society at large, such as being able to comprehend and write effective scientific articles, make effective presentations, and give and receive clear instructions.
7. **Individual and team work:** Think critically and work independently, and as a member or leader in diverse teams, and in multidisciplinary settings.
8. **Project management and finance:** Demonstrate knowledge and understanding of the scientific and management principles and apply these to one's own work, as a member and leader in a team, to manage projects and in multidisciplinary environments
9. **Ethics:** Apply ethical principles and commit to professional ethics and responsibilities and norms of scientific practice.
10. **The scientist and society:** Apply reasoning through the contextual knowledge to assess societal, health, safety, legal and cultural issues and the consequent responsibilities relevant to the professional scientific practice.
11. **Environment and sustainability:** Understand the impact of scientific processes in societal and environmental contexts, and demonstrate the knowledge, and need for sustainable development.
12. **Life-long learning:** Recognize the need for and have the preparation and ability to engage in independent and life-long learning in the broadest context of scientific and technological changes for up-to-date research and teaching methods.

## **Programme Specific Outcomes:**

- PSO1. Students will be capable of acquiring proficiency in interdisciplinary topics such as mathematics, and physics and the concepts needed for a proper understanding of Chemistry.
- PSO2. Students will demonstrate knowledge of Inorganic, Organic, Physical and Analytical Chemistry topics and be able to apply this knowledge to analyze a variety of chemical processes
- PSO3. Students will show that they have learned laboratory skills, enabling them to perform experiments in a chemical laboratory and analyze the measurements to draw valid conclusions. In addition, students will demonstrate skills in solving problems numerically using computer programming, plotting tools, and related software.
- PSO4. Students will demonstrate oral and written scientific communication and will demonstrate that they can think critically and work independently as well as in a team and play beneficial role in the society as a person of science combined with value-based education, both in professional and personal lives.

**MASTER OF SCIENCE**  
**CHEMISTRY**  
**M Sc Chemistry**  
**For 2018 admissions onwards**  
**GENERAL INFORMATION**

**Code Numbering:**

Each course is assigned an 8-character Code number. The first two digits indicate the year of curriculum revision. The next three letters indicate the Department offering the course. The last three digits are unique to the course – the first digit indicates the level of the course (100, 200, 300, 400 etc.); the second digit indicates the type of the course, viz. 0, 1 and 2 indicate the core courses; 3,4,5,6 and 7 indicate the Elective courses; 8 indicates the Lab. or practical-based courses and 9 indicates Projects.

**ABBREVIATIONS USED IN THE CURRICULUM:**

Cat - Category  
Cr - Credits  
ES - Exam Slot  
L - Lecture  
P - Practical  
T - Tutorial

**DISCIPLINES**

AVP - Amrita Values Programmes  
BUS - Business Management  
CHY - Chemistry  
CMJ - Communication and Journalism  
COM - Commerce  
CSA - Computer Science and Applications  
CSN - Computer Systems and Network  
CUL - Cultural Education  
ECO - Economics  
ELL - English Language and Literature  
ENG - English  
ENV - Environmental Sciences  
FNA - Fine Arts  
HIN - Hindi  
KAN - Kannada  
LAW - Law  
MAL - Malayalam  
MAT - Mathematics  
MCJ - Mass Communication and Journalism  
OEL - Open Elective  
PHY - Physics  
SAN - Sanskrit  
SSK - Soft Skills

SWK - Social Work

TAM - Tamil

## CURRICULUM

Course Code	Course Title	L T P	Cr	ES	Course Code	Course Title	L T P	Cr	ES
<b>SEMESTER 1</b>					<b>SEMESTER 2</b>				
18CHY501	Quantum Chemistry	3 0 0	3		18CHY511	Chemical Thermodynamics and Equilibria	3 1 0	4	
18CHY505	Group Theory and its Applications	0 0 0	3		18CHY512	Molecular Spectroscopy	3 1 0	4	
18CHY502	Concepts in Inorganic Chemistry	3 1 0	4		18CHY513	Organic Reaction Mechanism	3 1 0	4	
18CHY503	Principles in Organic Chemistry	3 0 0	3		18CHY514	Heterocyclic and Natural Products Chemistry	3 0 0	3	
18CHY504	Coordination Chemistry	3 0 0	3		18CHY515	Organometallic Chemistry	3 0 0	3	
18CHY581	Inorganic Semi-micro Qualitative Analysis Lab.	0 0 5	2		18CHY583	Advanced Physical Chemistry Lab.	0 0 5	2	
18CHY582	Organic Quantitative Analysis Lab.	0 0 5	2		18CHY584	Inorganic Quantitative Analysis Lab.	0 0 5	2	
18CUL501	Cultural Education	2 0 0	P/F		18AVP501	Amrita Values Programme	1 0 0	1	
<b>TOTAL</b>			<b>20</b>		<b>TOTAL</b>			<b>23</b>	
<b>SEMESTER 3</b>					<b>SEMESTER 4</b>				
18CHY601	Electrochemistry, Kinetics and surface Chemistry	3 1 0	4		18CHY696	Dissertation		14	
18CHY602	Synthetic Strategies and Reagents	3 1 0	4		<b>TOTAL</b>			<b>14</b>	
18CHY603	Solid State Chemistry and Materials Science	3 0 0	3						
18CHY604	Bioinorganic Chemistry	3 0 0	3						
	Elective	3 0 0	3						
18CHY681	Organic Qualitative Analysis Lab.	0 0 5	2						
18CHY682	Instrumental and Analytical Methods Lab.	0 0 5	2						
18CHY699	Project/seminar								
18CHY690	Live-in-Lab.@ / Open Elective*	2 0 0	2						
<b>TOTAL</b>			<b>23</b>		<b>TOTAL</b>			<b>80</b>	
<b>Electives</b>					<b>Open Electives</b>				
					<b>(2 0 0 2)</b>				
18CHY631	Applied Electrochemistry	3 0 0	3	E	18OEL631	Advanced Statistical Analysis for Research			
18CHY632	Bioanalytical Chemistry	3 0 0	3	E	18OEL632	Basics of PC Software			
18CHY633	Chemistry of Biomolecules	3 0 0	3	E	18OEL633	Computer Hardware and Networking			
18CHY634	Industrial Chemistry	3 0 0	3	E	18OEL634	Consumer Protection Act			
18CHY635	Industrial Stoichiometry	3 0 0	3	E	18OEL635	Corporate Communication			
18CHY636	Material Science and Nanochemistry	3 0 0	3	E	18OEL636	Design Studies			

18CHY637	Medicinal Chemistry	3 0 0	3	E	18OEL637	Disaster Management
18CHY638	Supramolecular Chemistry	3 0 0	3	E	18OEL638	Essentials of Cultural Studies
18CHY639	Nanomaterials for Biomedical Applications	3 0 0	3	E	18OEL639	Foundations of Mathematics
18CHY640	Industrial Metal Finishing Processes	3 0 0	3	E	18OEL640	Foundations of Quantum Mechanics
18CHY645	Analytical Methods			E	18OEL641	Glimpses of Life through Literature
18CHY641	Biosensors: Fundamentals and Applications	3 0 0	3	E	18OEL642	Information Technology in Banking
18CHY642	Computational Chemistry	3 0 0	3	E	18OEL644	Knowledge Management
18CHY643	Sustainable Chemical Science	3 0 0	3	E	18OEL645	Marketing Research
18CHY644	Sustainable techniques in Chemical Science	3 0 0	3	E	18OEL646	Media for Social Change
					18OEL647	Media Management
					18OEL648	Object-Oriented Programming
					18OEL649	Painting and Sculpture
					18OEL650	Personal Finance
					18OEL651	Principles of Advertising
					18OEL652	Principles of Packaging
					18OEL653	Scripting for Rural Broadcasting
					18OEL654	Social Media Website Awareness
					18OEL655	Theatre Studies
					18OEL656	Writing for Technical Purposes
					18OEL657	Yoga and Personal Development
					18OEL658	Fundamentals of Legal Awareness
					18OEL659	Solid Waste Management and Utilization
					18OEL660	Relativistic Quantum Mechanics
					18OEL661	Robotics and Biology
					18OEL662	Science of Well Being
					18OEL663	Operating Systems and Networks
					18EN600	Technical Writing
					18OEL664	Bhagavat Geeta and Personality Development
					18OEL665	Chemical Aspects of Forensic Science

## Evaluation Scheme and Grading System

### R.13 Assessment Procedure

R.13.1 The academic performance of each student in each course will be assessed on the basis of Internal Assessment (including Continuous Assessment) and an end-semester examination.

Normally, the teachers offering the course will evaluate the performance of the students at regular intervals and in the end-semester examination.

R.13.2 In theory courses (that are taught primarily in the lecture mode), the weight for the Internal Assessment and End-semester examination will be 50:50. The Internal assessment in theory courses shall consist of at least two periodical tests, weekly quizzes, assignments, tutorials, viva-voce etc. The weight for these components, for theory-based courses shall be 20 marks for the Continuous assessment, comprising of Quizzes, assignments, tutorials, viva-voce, etc. and 15 marks each for both the Periodical Tests.

At the end of the semester, there will be an end-semester examination of three hours duration, with a weight of 50 marks, in each lecture-based subject.

R.13.3 In the case of laboratory courses and practical, the relative weight for internal assessment and End-semester examination will be 80:20. The weight for the components of internal assessment will be decided by the course committee/class committee at the beginning of the course.

Evaluation pattern for course having both Theory and Lab components:

Courses having only one hour per week for lecture/tutorial, be treated as a Lab. course, for evaluation purposes; and evaluation pattern will be 80 marks for continuous assessment of lab work and 20 marks for end-semester lab examination.

Courses having two hours per week for theory and/or tutorials, be given a weight of 60 marks and 40 marks for the Theory and Lab components, respectively; The Lab. component evaluation will be based on continuous evaluation, without any end-semester practical evaluation. 10 marks will be for continuous assessment of the theory portion, 10 marks for each of the two periodical tests, 30 marks for the theory end-semester examination and 40 marks for continuous assessment of lab work and

Courses having three hours per week for theory and/or tutorials, be given a weight of 70 marks and 30 marks for the Theory and Lab components, respectively; The Lab component evaluation will be based on continuous evaluation, without any end-semester practical evaluation. 15 marks will be for continuous assessment of the theory portion, 10 marks for each of the two periodical tests, 35 marks for the theory end-semester examination and 30 marks for continuous assessment of lab work.

R.13.4 It is mandatory that the students shall appear for the end-semester examinations in all theory and weight courses, for completion of the requirements of the course. Those who do not appear in the end-semester examinations will be awarded 'F' grade, subject to meeting the attendance requirement.

At the end of a semester, examinations shall be held for all the subjects that were taught during that semester and those subjects of the previous semester s for which the student s shall apply for supplementary examination, with a prescribed fee.

R.13.5 PROJECT WORK: The continuous assessment of project work will be carried out as decided by the course committee. At the completion of the project work, the student will submit a bound volume of the project report in the prescribed format. The project work will be evaluated by a team of duly appointed examiners.

The final evaluation will be based on the content of the report presentation by student and a viva-voce examination on the project. There will be 40% weight for continuous assessment and the remaining 60% for final evaluation.

If the project work is not satisfactory he/she will be asked to continue the project work and appear for



assessment later.

#### R.14 PUBLICATION / INTERNSHIP

R.14.1 All students, if they are to be considered for award of the Degree at the time of graduation, are required to have published ONE paper in Scopus-indexed Journal/Conference.

R.14.2 Additional 5-10 marks will be awarded for each Publication, subject to a maximum of ONE paper per semester.

The additional marks shall be awarded in the semester in which the paper is published or accepted for publication, if applied for, within 10 days of the publication of results of the concerned semester. The additional marks can be awarded to any course(s) where the student has to improve his/her grade.

R.14.3 All publications shall be in Scopus-indexed Journals/Conferences and shall be as per the guidelines prescribed by the University.

R.14.4 Students who have undergone Internship at reputed organizations or National / International Institutions, with the prior approval of the concerned Departmental Chairperson and the Head of the School, may be considered for waiver of the requirement of publication, for the award of Distinction. However, the decision of the Departmental Chairperson and the Head of the School, in this regard, shall be final.

#### R.16 Grading

R.16.1 Based on the performance in each course, a student is awarded at the end of the semester, a letter grade in each of the courses registered.

Letter grades will be awarded by the Class Committee in its final sitting, without the student representatives. The letter grades, the corresponding grade points and the ratings are as follows:

Letter Grade	Grade Points	Ratings
0	10.00	Outstanding
A+	9.50	Excellent
A	9.00	Very Good
B+	8.00	Good
B	7.00	Above Average
C	6.00	Average
P	5.00	Pass
F	0.00	Fail
FA	0.00	Failed due to insufficient attendance
I	0.00	Incomplete (awarded only for Lab courses/ Project / Seminar)
W		Withheld

R.16.2 'FA' grade once awarded stays in the record of the student and is replaced with the appropriate grade when he/she completes the course successfully later.

Students who have secured an 'FA' in a course must re-register for the course or register for the course, if offered, under run-time re-do mode.

R.16.3 A student who has been awarded 'I' Grade in a Lab course, due to reasons of not completing the Lab., shall take up additional Lab. whenever offered next and earn a pass grade, which will be reflected in the next semester's grade sheet.

The 'I' grade, awarded in a Project/Seminar course, will be subsequently changed into appropriate grade,

when the student completes the requirement during the subsequent semester. If he/she does not complete it in the next semester, it will be converted to 'F' grade.

R.16.4 A student is considered to have successfully completed the course and earned the credit, if he/she scores a letter grade 'P' or better in that course.

#### R.21 Semester Grade Point Average (SGPA)

On completion of a semester, each student is assigned Semester Grade Point Average (SGPA) which is computed as below for all courses registered by the student during that semester.

$$\text{Semester Grade Point Average} = \frac{\sum (C_i \times G_{pi})}{\sum C_i}$$

where  $C_i$  is the credit for  $i$ th course in that semester and  $G_{pi}$  is the grade point for that course.

The summation is over all the courses registered by the student during the semester, including the failed courses. The SGPA is rounded off to two decimals.

#### R.22 Cumulative Grade Point Average (CGPA)

The overall performance of a student at any stage of the Degree programme is evaluated by the Cumulative Grade Point Average (CGPA) up to that point of time.

$$\text{Cumulative Grade Point Average} = \frac{\sum (C_i \times G_{pi})}{\sum C_i}$$

where  $C_i$  is the credit for  $i$ th course in any semester and  $G_{pi}$  is the grade point for that course.

The summation is over all the courses registered by the student during all the semesters up to that point of time, including the failed courses. The CGPA is also rounded off to two decimals.

#### R.23 Ranking

The ranking of the students in a batch at any intermediate or final stage is based on CGPA. Only those students who have passed all courses up to that stage in the first attempt are considered for ranking. Students are eligible for final ranking, only if the programme is completed within the normal duration, i.e., within two years from joining the programme.

#### R.24 Classification of successful candidates:

R.24.1 A student shall be considered to have successfully completed the programme, if he/she has:

- i) registered and successfully completed all the core courses, electives and projects as mentioned in the curriculum;
- ii) earned the required minimum number of credits as specified in the curriculum corresponding to the programme, within the stipulated time;
- iii) published a paper at a Scopus-indexed Journal/Conference.

R.24.2 Candidates who have successfully completed the programme, within a period of four semesters from entering the programme, shall be classified as follows:

Candidates securing a CGPA of 8.00 and above – FIRST CLASS WITH DISTINCTION \*

Candidates securing a CGPA between 6.50 and 7.99 – FIRST CLASS

and the same be mentioned in the Degree certificate;

(\*subject to satisfying the condition mentioned at R.14.1 and having passed all the courses, in the first attempt, in four semesters, from the date of joining the programme)

If the programme is completed after four semesters of study, the candidates securing even a CGPA of 8.00 and above, shall be classified to have completed the programme, only with FIRST CLASS.



## Course Objectives, Course Outcomes, Syllabus

18AVP201/ 18AVP211	Amrita Values Programme I/ Amrita Values Programme II	1 0 0 1 1 0 0 1
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### Objectives

The student will gain understanding of the glory of Indian Itihasa (Epics) in general, wherefrom the student get inspired to follow the lifestyle of inspiring characters depicted in Ramayana.

### Course Outcomes

After the completion of the course the student will be able to:

**CO 1:** Appreciate the relevance of Ramayana in modern times.

**CO 2:** Understand the family values and ideal human relationships portrayed in the Ramayana.

**CO 3:** Understand Dharma and its universality, emphasizing its applicability in an individual's life.

**CO 4:** Evaluate one's own personal ethics based on benchmarks from the Ramayana

**CO 5:** Apply the spiritual values from Ramayana in resolving personal and social conflicts.

**CO 6:** Understand the impact of itihisas on Indian civilization with reference to Mahabharata.

**CO 7:** Appreciate the relevance of Mahabharata and Bhagavad-Gita in the modern world.

**CO 8:** Understand the four goals of life (Purusharthas) as presented in the Mahabharata.

**CO 9:** Assimilate the positive qualities of the characters depicted in the itihasa.

**CO 10:** Analyse critical events and turning points in the Mahabharata with emphasis on the underlying values and principles.

### *Courses offered under the framework of Amrita Values Programmes I and II*

*Students shall have to register for any two of the following courses, one each in the third and the fourth semesters, which may be offered by the respective school during the concerned semester.*

### **Message from Amma's Life for the Modern World**

Amma's messages can be put to action in our life through pragmatism and attuning of our thought process in a positive and creative manner. Every single word Amma speaks and the guidance received in on matters which we consider as trivial are rich in content and touches the very inner being of our personality. Life gets enriched by Amma's guidance and She teaches us the art of exemplary life skills where we become witness to all the happenings around us still keeping the balance of the mind.

### **Lessons from the Ramayana**

Introduction to Ramayana, the first Epic in the world – Influence of Ramayana on Indian values and culture – Storyline of Ramayana – Study of leading characters in Ramayana – Influence of Ramayana outside India – Relevance of Ramayana for modern times.

### **Lessons from the Mahabharata**

Introduction to Mahabharata, the largest Epic in the world – Influence of Mahabharata on Indian values and culture – Storyline of Mahabharata – Study of leading characters in Mahabharata – Kurukshetra War and its significance - Relevance of Mahabharata for modern times.

### **Lessons from the Upanishads**

Introduction to the Upanishads: Sruti versus Smṛti - Overview of the four Vedas and the ten Principal Upanishads - The central problems of the Upanishads – The Upanishads and Indian Culture – Relevance of Upanishads for modern times – A few Upanishad Personalities: Nachiketas, Satyakama Jabala, Aruni, Shvetaketu.

### **Message of the Bhagavad Gita**

Introduction to Bhagavad Gita – Brief storyline of Mahabharata - Context of Kurukshetra War – The anguish of Arjuna – Counsel by Sri. Krishna – Key teachings of the Bhagavad Gita – Karma Yoga, Jnana Yoga and Bhakti Yoga - Theory of Karma and Reincarnation – Concept of Dharma – Concept of Avatar - Relevance of Mahabharata for modern times.

### **Life and Message of Swami Vivekananda**

Brief Sketch of Swami Vivekananda’s Life – Meeting with Guru – Disciplining of Narendra - Travel across India - Inspiring Life incidents – Address at the Parliament of Religions – Travel in United States and Europe – Return and reception India – Message from Swamiji’s life.

### **Life and Teachings of Spiritual Masters India**

Sri Rama, Sri Krishna, Sri Buddha, Adi Shankaracharya, Sri Ramakrishna Paramahansa, Swami Vivekananda, Sri Ramana Maharshi, Mata Amritanandamayi Devi.

### **Insights into Indian Arts and Literature**

The aim of this course is to present the rich literature and culture of Ancient India and help students appreciate their deep influence on Indian Life - Vedic culture, primary source of Indian Culture – Brief introduction and appreciation of a few of the art forms of India - Arts, Music, Dance, Theatre.

### **Yoga and Meditation**

The objective of the course is to provide practical training in YOGA ASANAS with a sound theoretical base and theory classes on selected verses of Patanjali’s Yoga Sutra and Ashtanga Yoga. The coverage also includes the effect of yoga on integrated personality development.

### **Kerala Mural Art and Painting**

Mural painting is an offshoot of the devotional tradition of Kerala. A mural is any piece of artwork painted or applied directly on a wall, ceiling or other large permanent surface. In the contemporary scenario Mural painting is not restricted to the permanent structures and are being done even on canvas. Kerala mural paintings are the frescos depicting mythology and legends, which are drawn on the walls of temples and churches in South India, principally in Kerala. Ancient temples, churches and places in Kerala, South India, display an abounding tradition of mural paintings mostly dating back between the 9th to 12th centuries when this form of art enjoyed Royal patronage. Learning Mural painting through the theory and practice workshop is the objective of this course.

### **Course on Organic Farming and Sustainability**

Organic farming is emerging as an important segment of human sustainability and healthy life. Haritamritam’ is an attempt to empower the youth with basic skills in tradition of organic farming and to revive the culture of growing vegetables that one consumes, without using chemicals and pesticides. Growth of Agriculture through such positive initiatives will go a long way in nation development. In Amma’s words “it is a big step in restoring the lost harmony of nature“.

### **Benefits of Indian Medicinal Systems**

Indian medicinal systems are one of the most ancient in the world. Even today society continues to derive enormous benefits from the wealth of knowledge in Ayurveda of which is recognised as a viable and sustainable medicinal tradition. This course will expose students to the fundamental principles and philosophy of Ayurveda and other Indian medicinal traditions.

### **Traditional Fine Arts of India**

India is home to one of the most diverse Art forms world over. The underlying philosophy of Indian life is ‘Unity in Diversity’ and it has led to the most diverse expressions of culture in India. Most art forms of India are an expression of devotion by the devotee towards the Lord and its influence in Indian life is very pervasive. This course will introduce students to the deeper philosophical basis of Indian Art forms and attempt to provide a practical demonstration of the continuing relevance of the Art.

### **Science of Worship in India**

Indian mode of worship is unique among the world civilisations. Nowhere in the world has the philosophical idea of reverence and worshipfulness for everything in this universe found universal acceptance as it in India. Indian religious life even today is a practical demonstration of the potential for realisation of this profound truth. To see the all-pervading consciousness in everything, including animate and inanimate, and constituting society to realise this truth can be seen as the epitome of civilizational excellence. This course will discuss the principles and rationale behind different modes of worship prevalent in India.

### **Temple Mural Arts in Kerala**

The traditional percussion ensembles in the Temples of Kerala have enthralled millions over the years. The splendor of our temples makes art enthusiast spellbound, warmth and grandeur of color combination sumptuousness of the outline, crowding of space by divine or heroic figures often with in vigorous movement are the characteristics of murals.

The mural painting specially area visual counterpart of myth, legend, gods, dirties, and demons of the theatrical world, Identical myths are popular the birth of Rama, the story of Bhīma and Hanuman, Shiva, as Kirata, and the Jealousy of Uma and ganga the mural painting in Kerala appear to be closely related to, and influenced by this theatrical activity the art historians on temple planes, wood carving and painting the architectural plane of the Kerala temples are built largely on the pan-Indians almost universal model of the Vasthupurusha.

### **Organic Farming in Practice**

Organic agriculture is the application of a set of cultural, biological, and mechanical practices that support the cycling of farm resources, promote ecological balance, and conserve biodiversity. These include maintaining and enhancing soil and water quality; conserving wetlands, woodlands, and wildlife; and avoiding use of synthetic fertilizers, sewage sludge, irradiation, and genetic engineering. This factsheet provides an overview of some common farming practices that ensure organic integrity and operation sustainability.

### **Ayurveda for Lifestyle Modification:**

Ayurveda aims to integrate and balance the body, mind, and spirit which will ultimately leads to human happiness and health. Ayurveda offers methods for finding out early stages of diseases that are still undetectable by modern medical investigation. Ayurveda understands that health is a reflection of when a person is living in harmony with nature and disease arises when a person is out of harmony with the cycles of nature. All things in the universe (both living and nonliving) are joined together in Ayurveda. This leaflet endow with some practical knowledge to rediscover our pre- industrial herbal heritage.

### **Life Style and Therapy using Yoga**

Yoga therapy is the adaptation of yogic principles, methods, and techniques to specific human ailments. In its ideal application, Yoga therapy is preventive in nature, as is Yoga itself, but it is also restorative in many instances, palliative in others, and curative in many others. The therapeutic effect comes to force when we practice daily and the body starts removing toxins and the rest is done by nature.

### **Insights into Indian Classical Music**

The course introduces the students into the various terminologies used in Indian musicology and their explanations, like Nadam, Sruti, Svaram – svara nomenclature, Stayi, Graha, Nyasa, Amsa, Thala,-

Saptatalas and their angas, Shadangas, Vadi, Samavadi, Anuvadi. The course takes the students through Carnatic as well as Hindustani classical styles.

### **Insights into Traditional Indian Painting**

The course introduces traditional Indian paintings in the light of ancient Indian wisdom in the fields of aesthetics, the Shadanga (Six limbs of Indian paintings) and the contextual stories from ancient texts from where the paintings originated. The course introduces the painting styles such as Madhubani, Kerala Mural, Pahari, Cheriya, Rajput, Tanjore etc.

### **Insights into Indian Classical Dance**

The course takes the students through the ancient Indian text on aesthetics the Natyasastra and its commentary the AbhinavaBharati. The course introduces various styles of Indian classical dance such as Bharatanatyan, Mohiniyattam, Kuchipudi, Odissi, Katak etc. The course takes the students through both contextual theory as well as practice time.

### **Indian Martial Arts and Self Defense**

The course introduces the students to the ancient Indian system of self-defense and the combat through various martial art forms and focuses more on traditional Kerala's traditional KalariPayattu. The course introduces the various exercise technique to make the body supple and flexible before going into the steps and techniques of the martial art. The advanced level of this course introduces the technique of weaponry.

### **Social Awareness Campaign**

The course introduces the students into the concept of public social awareness and how to transmit the messages of social awareness through various media, both traditional and modern. The course goes through the theoretical aspects of campaign planning and execution.

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leaflet endow with some practical knowledge to rediscover our pre- industrial herbal heritage.

### **Life Style and Therapy using Yoga**

Yoga therapy is the adaptation of yogic principles, methods, and techniques to specific human ailments. In its ideal application, Yoga therapy is preventive in nature, as is Yoga itself, but it is also restorative in many instances, palliative in others, and curative in many others. The therapeutic effect comes to force when we practice daily and the body starts removing toxins and the rest is done by nature.

**Learning Outcomes:** Amrita University's Amrita Values Programme (AVP) is a new initiative to give exposure to students about richness and beauty of Indian way of life. India is a country where history, culture, art, aesthetics, cuisine and nature exhibit more diversity than nearly anywhere else in the world. Amrita Values Programmes emphasize on making students familiar with the rich tapestry of Indian life, culture, arts, science and heritage which has historically drawn people from all over the world.

## **Evaluation Pattern – R.13 & R.16**

**18CHY501**

**QUANTUM CHEMISTRY**

**3 0 0 3**

### **Course Outcomes**

After completing the course, students will acquire

**CO 1:** Knowledge on origin of quantum mechanics, postulates of quantum mechanics and Schrodinger wave equation

**CO 2:** Knowledge on application of Schrodinger wave equation to various systems such as particle in a one-dimensional box and in a three-dimensional box, harmonic oscillator, rigid rotator, particle on a ring, and hydrogen atom and hydrogen-like species

**CO 3:** Knowledge and application of approximation methods such as independent particle model, variation method, perturbation method, and self-consistent field methods

**CO 4:** Application of quantum mechanics in chemical bonding – hydrogen molecule, hydrogen molecule ion, molecular orbital and valence bond theory, directed valences and hybridisation, band theory of metallic solids

**CO 5:** A knowledge on the different methods in computational quantum chemistry – molecular mechanics, molecular dynamics, semi-empirical, ab-initio, and DFT

**CO 6:** Theory and application of HMO and EHMO

### **Course Contents:**

#### **Unit I: Quantum Chemistry - Introduction**

Origin of quantum mechanics, de Broglie relationship, the uncertainty principle (no derivation); Postulates of quantum mechanics: postulate I – wave functions, postulate II- Operators in quantum mechanics, operator algebra, postulate-III – eigen values, eigen value equations, postulate IV – Expectation value, postulate V – time dependent and time independent Schrodinger equation.

#### **Unit II: Applying Schrodinger equation to various general systems**



Translational motion of a quantum entity (particle in one dimensional box and three dimensional box); vibrational motion (harmonic oscillator); rotational motion (rigid rotator, particle on a ring and particle on a sphere); angular momentum.

### **Unit III: Atomic structure and chemical bonding**

Hydrogen and hydrogen-like atoms; Multi electron systems- variation methods, perturbation methods, application to the ground state of Helium atom, SCF method, the exclusion principle

Chemical bonding: Hydrogen molecule ion and hydrogen molecule - molecular orbital and valence bond theory, homo and hetero nuclear diatomic molecules from VB and MO theory, the concept of directed valences and hybridization; quantum mechanics in band theory of metallic solids

### **Unit IV: Electronic structure of polyatomic systems: Computational quantum chemistry**

Semi empirical and ab-initio methods; QM approximations, Details of HMO and EHMO and its application to chemical bonding in unsaturated molecules(ethylene, 1,3butadiene etc) ; Details of SCF procedure, Hartree and Hartree Fock methods (up to ground and excited states of hydrogen molecule); the basis sets, STOs and GTOs, nomenclature of basis sets, basis set errors, introductory ideas on DFT.

### **Unit V: Molecular properties: Computational quantum chemistry**

Calculations of molecular properties like atomic charges, dipole moments, electronic distributions, vibration frequencies, NMR chemical shift etc using Gaussian program, specification of molecular geometry using Cartesian coordinates and internal coordinates, Z-matrix, Z-matrix of some simple molecules, structure of a Gaussian input file

### **TEXTBOOKS:**

1. *Ira N. Levin, 'Quantum Chemistry', 6<sup>th</sup> Edition, Prentice-Hall, 2008*
2. *Peter Atkins, Ronald Friedman, 'Molecular Quantum Mechanics', 4<sup>th</sup> edition, Oxford university press*
3. *R K Prasad, 'Quantum Chemistry', New Age International (P) LTD publishers*

### **REFERENCES:**

1. *Andrew R Leech, 'Molecular Modeling – Principles and Applications', 2<sup>nd</sup> Edition, Pearson Education.*
2. *Donald A. McQuarrie, 'Quantum Chemistry', Viva Books 2016.*

**Learning Outcomes:** In this course students learn the basics of quantum chemistry and its application in various types of the systems. This knowledge is essential for the students to continue their studies in chemistry and to seek a profession related to chemistry.

## **Evaluation Pattern – R.13 & R.16**

18CHY502

Concepts in Inorganic Chemistry

3 1 0 4

### **Course Outcomes**

After completion of the course, students will be

**CO 1:** Able to qualitatively interpret a decay series and compare the penetrating power of alpha, beta, neutron, and gamma radiation

**CO 2:** Able to understand the factors that determine the biological effects of radiation.

**CO 3:** Able to criticize how nuclear chemistry and radiochemistry methods can be used to make issues more visible and solve problems, particularly in relation to environmental problems and metal production.

**CO 4:** Aware of the contributions of chemistry to society, interaction of radiation with matter and improve their knowledge of instrumentation and introduction to health – physical applications in nuclear and radiochemistry.

**CO 5:** Able to explain new functional materials like fullerenes, carborenes, crown ethers etc. and their applications.

**CO 6:** Able to predict the structure based on Styx numbers.

**CO 7:** Able to draw the structures of inorganic chains and polymers and the different silicate structures.

**CO 8:** Able to differentiate pseudo halogen and inter halogen compounds and their applications.

**CO 9:** Able to correlate electronic, magnetic and optical properties with the electronic structures of the 4f elements.

**CO 10:** Able to compare the properties of lanthanides and actinides and also get a general awareness of mineral wealth of our country.

### **Course Contents:**

#### **Unit 1 Nuclear Chemistry**

Nuclear structure, mass and charge, mass defect, binding energy, stability rules, magic numbers, nuclear quantum numbers, nuclear parity and statistics, models of nucleus, shell model, liquid drop model, semi empirical mass equation, equations of radioactive decay and growth, half-life, average life determination of half-lives, nuclear reactions, energetics of nuclear reactions, types of nuclear reactions, spontaneous and induced fission, neutron capture cross sections- critical size principle and working of nuclear reactor. Numerical problems relevant to each session.

#### **Unit 2 Radiation Chemistry**

Radioactive elements, decay kinetics, parent-daughter decay relationships, radioactive equilibrium - transient and secular equilibrium, alpha and beta decay, gamma emission, Radiochemical methods - measurement of radioactivity, measurement of radiations - ionization chamber, proportional counter, the Geiger counter, scintillation counter, semiconductor detectors. Applications of nuclear and radiation chemistry, isotope dilution analysis - activation analysis, radioactive tracers, radiometric titrations, radiation dosimetry, hydrated electron.

#### **Unit 3 Inorganic materials I**

Alkali and alkaline earth metals, their compounds, crown ethers and cryptands as complexing agents for alkali metal ions, Be and Mg compounds, boron cage compounds, boron hydrides, structure and bonding, 3-centre-2-electron bonds, styx numbers, the importance of icosahedral frame work of boron atoms in boron chemistry, closo, nido and arachno structure, carboranes, metallocene carboranes, B-N compounds, interstitial compounds, metal carbides, nitrides and hydrides, fullerenes, functionalized fullerenes, C-nanotubes.

#### **Unit 4 Inorganic materials II**

Inorganic chains and polymers, rings, cages, and clusters, sulphur-nitrogen compounds, polymeric sulphur nitride, isopoly anions, heteropoly anions, Keggin and Dawson polyoxometallates, borazines, metal clusters, nature of Si-Si bonds, silicates, silicates with zero-, one-, two- and three-dimensional structures, structure of elemental P, phosphonitrilic compounds, polymers with P-N bonds, interhalogen and pseudo halogens, intercalation chemistry, intercalation in layered materials like graphite, xenon fluorides & other xenon compounds.

## Unit 5 Chemistry of f-block elements

The lanthanides and actinides, stable oxidation states, the lanthanide and actinide contractions, the f-orbitals, spectral and magnetic properties - comparison with inner transition and transition metals, separation of lanthanides, use of lanthanide compounds as shift reagents, photo-emission of lanthanide compounds, organometallic compounds of lanthanides and actinides and their structural features, reactions of lanthanide and actinide compounds, mineral sands of south west India - Ilmenite, Monazite, etc.

### TEXTBOOKS:

1. H J Arnikaar, Essentials of Nuclear Chemistry, 4<sup>th</sup> revised edition, New Age International (P) Limited publishers, 2015.
2. H J Arnikaar, Nuclear Chemistry through Problems, New Age International Publishers.
3. J. Huheey, Inorganic Chemistry: Principles of Structure and Reactivity, 4<sup>th</sup> edition, 2006.
4. F.A. Cotton, Advanced Inorganic Chemistry, Wiley; 6th Edition edition (22 April 1999)
5. J.D. Lee Concise Inorganic Chemistry, Oxford University Press, 5<sup>th</sup> edition, 2008

### REFERENCES:

1. Gregory R. Choppin, Jan-Olov Liljenzin and Jan Rydberg, Radiochemistry and Nuclear Chemistry (Third Edition), Elsevier, 2002
2. Walter D. Loveland, David J. Morrissey, Glenn T. Seaborg, Modern nuclear chemistry, A JOHN WILEY & SONS, INC., PUBLICATION, 2017.
3. Shriver and Atkins' Inorganic Chemistry, Oxford; 5 edition, 2009.

**Learning Outcomes:** In this course students learn the basics of nuclear and radiochemistry and their applications along with the structures and applications of functional materials like fullerenes, carborenes, crown ethers etc. They will also get to learn about the properties of lanthanides and actinides and their applications. This knowledge is essential for their progress in chemistry related courses and/or jobs.

## Evaluation Pattern – R.13 & R.16

18CHY503

Principles in Organic Chemistry

3 0 0 3

### Course Outcomes

After completing the course, students will

**CO 1:** Understand the concepts of aromaticity and field effects

**CO 2:** Understand and reproduce accepted mechanisms of organic reactions including all intermediates, arrows, charges, and resonance structures.

**CO 3:** Be able to draw all the stereoisomers of organic compound and recognise enantiomers, diastereomers, meso compounds

**CO 4:** become familiar with the relative stability of conformational isomers of cyclohexanes and related compounds.

**CO 5:** Be able to predict the major and minor products of a variety of organic reactions with appropriate stereochemistry and regio-chemistry.

### Course Contents:

**Unit 1 Aromaticity:** Review of inductive and field effects – Resonance effects. Criteria for aromaticity – structural and electronic. Types – Huckel and Craig's rule, homo (Five, Six, seven and eight, membered rings), hetero (furan, thiophene and pyrrole) and nonbenzenoid aromatic systems. Aromaticity of fused rings, annulenes, catenanes, rotaxanes, mesoionic compounds, metallocenes, cyclic carbocations and carbanions.

**Unit 2 Structure activity relationships** – Orientation effects of substituent, Quantitative treatment of structure on reactivity - free energy relationships – Hammett equations, Taft equation.

Reactive Intermediates: Generation, structure and reactivity - reactions and rearrangement involving) of carbocations - non-classical carbocations, carbanions, carbon radicals, radical ions, carbenes, nitrenes, isonitrenes, arynes.

**Unit 3 Mechanism and methods to determining them:** Thermodynamic and kinetic requirement, Baldwin rules for ring closure – Kinetic and thermodynamic control – Hammond postulates, microscopic reversibility, Marcus theory, methods of determining reaction mechanisms - solvents and their effect on course of a reaction.

Acids and Bases: Bronsted and Lewis acids - HSAB concept and bases, pH and pKa, effect of structure on acidity and basicity, effect of medium.

#### **Unit 4 Stereochemistry**

Optical and geometrical isomerism, absolute and relative configuration, Cahn-Ingold-Prelog system, prochirality, prochiral centre, atoms, groups and faces, designations. Atropisomerism, optical isomerism in biphenyls, allenes, spirans and “ansa” compounds, compounds containing chiral nitrogen and sulfur atom, geometrical isomerism of cyclic compounds, cumulenes and oximes. Asymmetric synthesis, stereospecific and stereoselective synthesis, regioselective and regiospecific reactions.

#### **Unit 5 Conformational Analysis**

Conformational analysis of cyclic and acyclic systems with special emphasis on six membered rings, conformational effects on the reactivity of acyclic and cyclic systems - elimination, substitution and addition, strain, structure and stability of small, medium, and large rings, anomeric effect - cycloalkenes and cycloalkynes - kinetically and thermodynamically favoured products stereochemistry of SN1, SN2, SNi, E1 and E2

**Selectivity in organic reactions:** Chemoselectivity, regioselectivity, enantio- and stereo-selectivity. Stereoaspects of the addition of X<sub>2</sub>, HX, boranes and hydroxylation to C=C systems. *Cis*- and *trans*-hydroxylation of cycloalkenes.

#### **TEXT BOOKS**

1. Michael B Smith, “March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure”, 7<sup>th</sup> edition, Wiley (2015).
2. Francis A. Carey and Richard J. Sundberg, “Advanced Organic Chemistry - Part A: Structure and Mechanisms”, 5<sup>th</sup> Edition, Springer, 2008
3. P. S. Kalsi, “Stereochemistry, Conformation and Mechanism”, New Age Publications, 2008.

#### **REFERENCES**

1. E. L. Eliel and S. H. Wilen, “Stereochemistry in Organic Compounds”, John Wiley, 2008.
2. D. Nasipuri, “Stereochemistry of Organic Compounds - Principles and Applications”, 4<sup>th</sup> Revised Edition, New Academic Science, 2012.
3. Peter Sykes, “A Guidebook to Mechanism in Organic Chemistry”, Pearson Education; 6<sup>th</sup> edition, 2003.

**Learning Outcomes:** In this course students learn about the concepts of organic chemistry, principles, theories, classifications, synthetic methods, structure and bonding, reaction mechanisms the applications of organic compounds in various fields. This knowledge is essential for the students to pursue their higher studies in chemistry and to seek a profession related to synthetic or analytical chemistry.

#### **Evaluation Pattern – R.13 & R.16**

18CHY504

Coordination Chemistry

3 0 0 3

#### **Course Outcomes**

After completing the course, the students will be in a position to

**CO 1:** Apply the various theories of coordinate bonding to predict the geometry and properties of

complexes.

**CO 2:** Interpret the electronic spectra and magnetic properties of complexes.

**CO 3:** Improve their analytical and critical thinking through the reaction mechanism and stereochemistry of reactions.

**CO 4:** Obtain a sound theoretical knowledge in bonding, reactivity and geometry of f-block metal coordination compounds.

### Course Contents:

#### Unit 1 Theories and Concepts on *d*-block Coordination Compounds

Introduction - ligands, nomenclature of coordination compounds, coordination compounds of *d*-block ions with coordination numbers of 2, 3, 4, 5, 6, 7 and 8. Werner's coordination theory, Valence bond theory (VBT), Crystal field theory (CFT), CFSE, effects of CFSE on hydration energies and spinel groups (normal and inverse), types of ligands – spectrochemical series, spectral and magnetic properties (spin-only magnetic moments), nephelauxetic effect. Crystal field splitting patterns in complexes having Oh, Td, square planar, square pyramidal and trigonal pyramid geometries, factors affecting the magnitude of CFSE, various types of isomerism in coordination complexes, Jahn-Teller (JT) distortion, manifestation of JT on spectral properties. Molecular orbital theory (MOT), ligand field theory (LFT), molecular orbital energy level diagram for octahedral complexes without pi-bonding, metal-ligand pi-bonding, metal-metal multiple bonds, *d*-orbital based metal-metal  $\sigma$ ,  $\pi$  and  $\delta$  bonds in compounds like  $[\text{Re}_2\text{Cl}_8]^{2-}$ ,  $[\text{Os}_2\text{Cl}_8]^{2-}$ ,  $\text{Cr}_2(\text{CH}_3\text{COO})_4$  and R-Cr(I)-Cr(I)-R. Application of group theory to coordination compounds.

#### Unit 2 Reaction Mechanism

Complex equilibrium - formation constants, chelate and macrocyclic effects, factors affecting stability of complexes, methods of determination of stability constants, stability of complex ions in solutions, inert and labile complexes, mechanisms of ligand displacement and addition reactions in octahedral complexes and square planar complexes of platinum *cis*- and *trans*-effect, substitution reactions, mechanisms of substitution, kinetic consequences of reaction pathways, dissociation, interchange, association, dissociation, linear free energy relationships, conjugate base mechanism, stereochemistry of reactions (substitution in *trans*-complexes and substitution in *cis*-complexes), isomerisation of chelate rings, sigma-bonding and pi-bonding effects, oxidation-reduction reactions, inner and outer sphere electron transfer reactions, conditions for high and low oxidation numbers, reactions of coordinated ligands, hydrolysis of esters, amides and peptides, template reactions, electrophilic substitution, photochemical reactions of coordination compounds.

#### Unit 3 Coordination Chemistry of Inner-transition (*f*-block) Elements

*f*-block metal ions – oxidation states preferences, ligand preferences, coordination numbers and the geometry of the complexes, influence of lanthanide contraction and actinide contraction in their coordination behaviour, shapes of *f*-orbitals (4*f* and 5*f*), nature of bonding of *f*-orbitals with ligands, various types of coordination compounds of lanthanides and actinides, stereochemistry and reaction mechanism of *f*-block metal complexes.

#### Unit 4 Spectral Properties

Stabilization of unusual oxidation states, electronic spectra of transition metal complexes – color wheel, Russell-Saunders coupling schemes, term symbols for various  $d^n$  ions, Orgel diagrams for  $d^n$  systems, ligand field parameters,  $Dq$ , Racah parameter  $B$  and nephelauxetic constant  $b$ , Tanabe-Sugano (TS) diagrams, evaluation of  $Dq$  and other parameters from electronic spectra of transition metal complexes using TS diagrams, charge-transfer transitions, MLCT and LMCT, selection rules and band intensities, Laporte- and spin- selection rules, symmetry, spin-orbit and vibronic coupling effects. Photochemistry of transition metal complexes like  $[\text{Ru}(\text{bipy})_3]^{2+}$ , spectral behaviour of *f*-block coordination complexes, special features of their absorption and emission properties.

#### Unit 5 Magnetic Properties

Magnetic properties of coordination complexes - magnetic susceptibility, contribution of spin-orbit

coupling on  $\mu_{\text{eff}}$ , types of magnetic behavior - para-, ferro, anti-ferro and ferri-magnetic systems, Curie law, Curie-Wise law, Guoy, Faraday and superconducting quantum interference device (SQUID) methods, Kotani plots, giant magnetoresistance (GMR), anisotropic magnetoresistance (AMR) effect, effects of temperature on magnetic behavior, tunneling magnetoresistance (TMR). Magnetism of coordination complexes by multinuclear homo- and heterometallic  $3d$  systems (also with exclusive  $4d$  and  $5d$  metal ions), mixed  $3d-4f$  systems, importance of  $4f$ -metal ions for functional applications. Nanoscale magnetic systems based on coordination complexes - Single Molecule Magnets (SMMs), Single Ion Magnets (SIMs), Single Chain Magnets (SCMs), Spin-crossover complexes, magnetic refringents (magnetic coolers), magnetic storage systems - magnetic random access memory (MRAM).

#### TEXTBOOKS:

1. F. A. Cotton and G. Wilkinson, 'Advanced Inorganic Chemistry', John Wiley & Sons, 2009.
2. James E. Huheey, Ellen A. Keiter and Richard L. Keiter, 'Inorganic Chemistry, Principles of Structure and Reactivity', Pearson education, 5th edition, 2009.
3. J. D. Lee, 'Concise Inorganic Chemistry', 5th edition, John Wiley & Sons, 2009.
4. P Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, "Shriver & Atkins Inorganic chemistry", 4th Edition, Oxford University Press, 2008.

#### REFERENCES:

1. B. Douglas, D. McDaniel and J. Alexander "Concepts and Models in Inorganic Chemistry", 3rd Edition, Wiley, 2006.
2. Sushanta Dattagupta, 'A Paradigm Called Magnetism', World Scientific Publishing Co. Pte. Ltd., 2008.
3. Helen C. Aspinall, 'Chemistry of the  $f$ -Block Elements', Volume 5 of Advanced chemistry texts, CRC Press, 2001.
4. N. N. Greenwood and A. Earnshaw, 'Chemistry of Elements', Butterworth and Heinemann, 2nd Edition, 2002
5. J. E. House, "Inorganic Chemistry", Academic Press, 2008.
6. T. Shinjo (Editor), 'Nanomagnetism and Spintronics', Elsevier, USA, 2<sup>nd</sup> Ed., 2014.
7. R. A. Layfield and M. Murugesu (Editors), 'Lanthanides and Actinides in Molecular Magnetism', Wiley-VCH Verlag & Co., 2015.

**Learning Outcomes:** In this course students learn about the concepts of coordination chemistry, theories, synthesis, bonding, structure, characterizations, functional properties and the applications of coordination compounds in various fields, like, medicine and catalysis. This knowledge is essential for the students to pursue their higher studies in inorganic chemistry and to seek a profession related to catalysis or medicinal chemistry.

#### Evaluation Pattern – R.13 & R.16

18CHY505

GROUP THEORY AND ITS APPLICATIONS

3 0 0 3

#### Course Outcomes

After completing the course, student gains

**CO 1:** A knowledge on basis sets and nomenclature of basis sets

**CO 2:** Specification of molecular geometry

**CO 3:** A knowledge in group in mathematics, elements of symmetry in molecules, symmetry operations, molecular point group, abelian and cyclic group.

**CO 4:** A knowledge in similarity transformation and classes of point group, group multiplication table, and Schoenflies symbols

**CO 5:** A knowledge in reducible and irreducible representations, great Orthogonality Theorem and its

consequences, and construction of character table for point groups

**CO 6:** A knowledge in the application of group theory to spectroscopy – IR and Raman activity of molecular vibrations, and electronic spectroscopy

**CO 7:** A knowledge in the application of group theory to chemical bonding – hybridisation, and molecular orbital formation

### Course Contents:

#### Unit I Introduction to molecular point groups

Definition of a mathematical group, Symmetry in molecules, elements of symmetry, , matrix representation of symmetry operations, molecular point groups, , abelian group, cyclic group, symmetry operations as group elements, similarity transformation and classes, group multiplication table, symmetry classification of molecules into pointgroups (Schoenflies symbol)

#### Unit II Construction and interpretation of character tables

Reducible and irreducible representations, Great Orthogonality Theorem and its consequences, character tables, reduction formula, construction of character tables for point groups with order  $\leq 6$ , interpretation of character tables.

#### Unit III Applications of Group theory - I (vibrational and electronic spectroscopy)

Infrared and Raman activity of molecular vibrations in  $\text{H}_2\text{O}$ ,  $\text{N}_2\text{F}_2$ ,  $\text{BF}_3$ ,  $\text{AB}_4$  type molecules ( $\text{Td}$  and  $\text{D}_{4h}$ ) and  $\text{AB}_6$  type ( $\text{O}_h$ ) of molecules; selection rules; Electronic structure of free atoms and ions, splitting of terms in a chemical environment, construction of energy level diagrams, estimations of orbital energies, selection rules and polarizations, double groups, a brief idea on electronic spectra of transition metal complexes – selection rules, Orgel diagrams, Tanabe Sugano diagrams.

#### Unit IV: Applications of Group theory (Chemical bonding - Hybridization and molecular orbital formation)

Group theory to explain hybridization - wave functions as bases for irreducible representations, construction of hybrid orbitals for  $\text{AB}_3$  (planar),  $\text{AB}_4$  ( $\text{Td}$ ),  $\text{AB}_5$  ( $\text{D}_{3h}$ ) and  $\text{AB}_6$  ( $\text{O}_h$ ) type of molecules, symmetry adapted linear combinations, projection operators, application of projection operators to pi-bonding in ethylene, cyclopropenyl systems and benzene, application of symmetry to predict polar and chiral compounds;

#### Unit V: Symmetry in solid state

Symmetry elements and operations in solid state – proper axis of rotation, mirror planes of symmetry, roto-reflection and roto-inversion axes of symmetry, screw axes of symmetry, glide planes; a brief introduction to the crystallographic point groups and space groups

#### TEXTBOOKS:

1. F. Albert Cotton, 'Chemical Applications of Group Theory', 3<sup>rd</sup> Edition, John Wiley, 1990.
2. A Salahuddin Kunju, G Krishnan ; 'Group theory and its application in chemistry', second edition, PHI Learning private limited-2015

#### REFERENCES:

1. Robert L Carter, 'Molecular symmetry and Group theory', John Wiley & Sons, Inc.
2. V. Ramakrishnan and M.S. Gopinathan, 'Group Theory in Chemistry', 2<sup>nd</sup> reprint edition, Vishal Publications, 1996.
3. P.H. Walton, "Beginning Group Theory for Chemistry", Oxford University Press Inc., New York, 1998.

**Learning Outcomes:** In this course students learn the basics of group theory and its application in various types of the systems in chemistry. This knowledge is essential for the students to continue their studies in chemistry and to seek a profession related to chemistry.

**18CHY511 CHEMICAL THERMODYNAMICS AND EQUILIBRIA 3 1 0 4**

**Course Outcomes**

The course helps students to gain

**CO 1:** Knowledge in equilibrium chemical thermodynamics

**CO 2:** Ability to apply theories and laws of equilibrium chemical thermodynamics

**CO 3:** A knowledge in irreversible thermodynamics

**CO 4:** A knowledge in statistical thermodynamics

**CO 5:** Ability to apply statistical thermodynamics to solve problems

**CO 6:** A knowledge on chemical and phase equilibria

**Course Contents:**

**Unit 1 Chemical Thermodynamics**

First and second laws of thermodynamics, thermodynamic functions, heat capacity, thermo chemistry, need for second law of thermodynamics, entropy and free energy functions, calculation of changes in thermodynamic function for ideal and non-ideal gases in isothermal and adiabatic process, relation between thermo dynamic functions - Maxwell relations, Joule Thomson effect, coefficient of thermal expansion and compressibility factor, applications of free energy function to physical and chemical changes, equilibrium in chemical reactions, third law of thermodynamics - need for third law, calculation of absolute entropy, unattainability of absolute zero, thermodynamic systems of variable composition - fugacity functions, partial molar quantities, thermodynamics of ideal solutions, real solutions and regular solutions, dilute solutions of nonelectrolytes, Henry's law, Raoult's law, Gibbs-Duhem equations, Gibbs-Duhem-Margules equations, and activity and standard states of non electrolytes.

**Unit 2 Irreversible Thermodynamics**

Examples for irreversible process, entropy production, non-equilibrium, steady state and near equilibrium conditions, linear relation, phenomenological coefficients, Onsagar reciprocal relations, one component systems with heat and matter transport, application of irreversible thermodynamics to thermal diffusion, thermal osmosis etc., electro kinetic effects, the Glansdorf-Pregogine equation.

**Unit 3 Statistical Thermodynamics**

Statistical concept, probability and thermodynamic states, entropy and probability, canonical ensemble, Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein Statistics, electron gas concept, Bose-Einstein condensation, relation among MB, FD & BE Statistics, partition function, partition function for free linear motion, free motion in a shared space, linear harmonic vibration, translational, rotational and vibrational partition function, molecular partition functions, partition functions and thermodynamic properties, calculation of equilibrium constant, heat capacity of gases, mono atomic solids, Einstein's and Deby's theory.

**Unit 4 Equilibrium**

Gibb's free energy, direction of spontaneous change of a reaction, chemical potential, chemical potential and equilibrium,  $\Delta G$  in terms of K, equilibrium constants – real gases and real reactions, equilibrium respond to catalyst, temperature, pressure and  $pH$ , application of  $\Delta G$  and K – extraction of metals from their oxides, Ellingham diagram, and thermodynamics of ATP & respiration, biological energy conversion.



## Unit 5 Phase Equilibrium

Gibb's Phase rule, one component system, two component systems, vapour pressure diagrams and their interpretation, lever rule, temperature-composition diagrams, liquid-liquid phase diagrams, distillation of partially miscible liquids, azeotropes, liquid-solid phase diagrams, phase diagram for the system Na/K/Na<sub>2</sub>K, phase diagram - steel, alloys, Fe-C system, zone refining, three component system, triangular coordinates, three component system – partially miscible liquids - H<sub>2</sub>O/CHCl<sub>3</sub>/CH<sub>3</sub>COOH, phase diagram - NH<sub>4</sub>Cl/(NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>/H<sub>2</sub>O

### TEXTBOOKS:

1. Robert J. Silbey, Robert A. Alberty, Mounji G. Bawendi, Physical Chemistry 4th Edition, Wiley, 2004
2. Samuel H. Maron, Carl F. Prutton Principles of Physical Chemistry, The Macmillan Company; 4th edition (1970)
3. Samuel Glasstone, 'Thermodynamics for Chemists', Lightning Source Incorporated, 2007.

### REFERENCES:

1. Francis Weston Sears and Gerhard L. Salinger, 'Thermodynamics, kinetic theory and statistical thermodynamics' 3<sup>rd</sup> edition, Addison-Wesley Publications, 1975.
2. Prigogine, 'Introduction to Thermodynamic Irreversible Processes', Interscience Publishers, 3<sup>rd</sup> edition, 1968.
3. R.P. Rastogi and R.R. Misra, 'An Introduction to Chemical Thermodynamics', 6<sup>th</sup> Revised edition, Vikas Publishing House Pvt. Ltd., 2006.
4. F.W. Sears, 'Introductions to Thermodynamics, Kinetic Theory of Gases and Statistical Mechanics', Addison Wesley Pub., Cambridge, 1972.

**Learning Outcomes:** In this course students learn about the various theories and concepts of thermodynamics and statistical thermodynamics as well as phase equilibrium. This knowledge is essential for the students to continue their studies in chemistry and to seek a profession related to chemistry.

## Evaluation Pattern – R.13 & R.16

18CHY512

MOLECULAR SPECTROSCOPY

3 1 0 4

### Course Outcomes

After the completion of the course, the students will have

**CO 1:** Thorough understanding of the fundamental theoretical concepts of spectroscopy, based on quantum chemistry, group theory and statistical thermodynamics.

**CO 2:** Thorough understanding of the fundamentals of instrumentation of spectroscopic techniques.

**CO 3:** Ability to apply the knowledge of spectroscopy to provide analytical solutions for problems of chemical interest.

### Course Contents:

#### Unit 1 Rotational and Vibrational Spectroscopy

Introduction to spectroscopy, rotation spectra - diatomic and polyatomic molecules, selection rules, intensities of spectral lines, Stark effect, instrumentation of micro wave spectroscopy, applications and structural determinations, vibration spectra of diatomic molecules, harmonic and anharmonic vibrations, diatomic vibrating rotor, selection rule, breakdown of Born Oppenheimer approximation, rotational character of vibration spectra, different modes of vibrations, vibration-rotation spectra, Fermi resonance,

vibration spectra of polyatomic molecules, IR spectra of organic and inorganic compounds, phase, temperature and solvent dependence, FTIR technique, instrumentation, Raman spectra (including the use of laser) - theory, relation with IR spectroscopy, mutual exclusion principle, resonance Raman, stimulated hyper and inverse Raman effects, instrumentation and applications of Raman spectroscopy.

## **Unit 2 UV-Visible and Fluorescence Spectroscopy**

Electronic spectra of atoms - single and multi electron systems, j-j and L-S coupling, electronic spectra of diatomic and polyatomic molecules, its relation to electronic arrangement and symmetry of molecules, application of group theory in electronic spectra, selection rules, nature of electronic excitation, principles of absorption spectroscopy, Beer-Lambert law, presentation of spectra, chromophores, forbidden transition, different types of electronic transitions, p-p\*, n-p\* etc transitions, nature of transitions in carbonyl compounds, the effect of conjugation, effect of conjugation on alkenes, HOMO and LUMO, Woodward-Fieser rules for dienes, spectra of carbonyl compounds, enones, Woodward rule for enones, spectra of aromatic compounds, effect of substituents, structural information from electronic spectra, excited states of molecules, fluorescence and phosphorescence, Jablonski diagram in detail, lifetime of excited states, quantum yields, photosensitization, application of UV-Visible and Fluorescence Spectroscopy for structural elucidation of organic compounds, diffuse reflectance spectra.

## **Unit 3 NMR Spectroscopy**

Nuclear magnetic resonance phenomenon - theory, relaxation effects, NMR uses active nuclei, Fourier Transformation in NMR, measurement of relaxation time, chemical shift, magnetic anisotropic effect, multiplets in NMR, spin-spin splitting, n + 1 rule, Pascal's triangle, tree-diagram, spin-spin splitting constant, J,  $^2J$  and  $^3J$  and long-range coupling, measurement of J, Karplus relationship, first and second order spectra, AX, AB, AX<sub>2</sub>, AX<sub>3</sub>, A<sub>2</sub>X<sub>3</sub>, AMX type spectra, double resonance and spin tickling, chemical shift reagents, spectra in higher fields, spectra of conformational isomers, homotopic, enantiotopic and diastereotopic systems, C<sup>13</sup> spectra, factors related to <sup>13</sup>C spectra, <sup>1</sup>H coupled <sup>13</sup>C spectra, <sup>1</sup>H decoupled <sup>13</sup>C spectra, chemical shift values, nuclear Overhauser effect (NOE), cross-polarization, off-resonance resonance decoupling, application of <sup>1</sup>H and <sup>13</sup>C NMR spectroscopy for the structural elucidation of organic compounds, <sup>11</sup>B, <sup>15</sup>N, <sup>19</sup>F and <sup>31</sup>P NMR spectra, spectra of paramagnetic complexes, magnetic susceptibility, contact shift, fluxional molecules and their studies using NMR, solid state NMR.

## **Unit 4 ESR, NQR and Mossbauer Spectroscopy**

ESR spectroscopy - theory, hyperfine and superfine splitting, ESR active simple organic systems, ESR of inorganic systems like Cu<sup>2+</sup> and VO<sup>2+</sup> complexes, 'g' markers like DPPH and TCNE, evaluation of spin Hamiltonian like A, g<sub>||</sub>, g<sub>⊥</sub>, covalency factor in Cu<sup>2+</sup> complexes, analysis of ESR spectra of VO<sup>2+</sup> complexes, NQR spectroscopy - theory, relationship between electric field gradient and molecular structure, quadrupole coupling constant and structural information of compounds, Mossbauer spectroscopy, principle, Doppler effect, isomer shift, Zeeman splitting, quadrupole splitting, application of Mossbauer spectroscopy for studying Fe and Sn compounds and phase transformation, application of ESR spectroscopy.

## **Unit 5 Mass Spectrometry and PES**

Mass spectroscopy, base peak and molecular ion peak, isotope ratio data, fragmentation patterns of alkanes, alkenes, alkynes, aromatic hydrocarbons, alcohols, phenols, aldehydes, ketones, esters, carboxylic acids, amines, methods of desorption and ionization (EI, CI, LD, MALDI, PD, FAB, SIMS), MS/MS and determination of molecular formula, metastable ions and their significance, study of fragmentation pattern, application of MS in structural elucidation and other frontiers of science, application of MS for quantitative analysis, photoelectron spectroscopy (PES), principle, application of PES. Structure determination using IR, UV-visible, NMR, MS and ESR spectral techniques.

### **TEXTBOOKS:**

1. Colin N. Banwell and Elaine M. McCash, 'Fundamentals of Molecular Spectroscopy', 4<sup>th</sup> Edition, Tata McGraw Hill, 2007.
2. W. Kemp, *Organic Spectroscopy*, 3<sup>rd</sup> Edition, McMillan International Higher Education
3. D. L. Pavia, G. M. Lampman, G. A. Kriz, and J. R. Vyvyan, *Introduction to Spectroscopy*, 5<sup>th</sup> Edition, Brooks-Cole, 2009
4. G. M. Barrow, 'Introduction to Molecular Spectroscopy', McGraw Hill, 1962.
5. R. M. Silverstein, F. X. Webster, D.J. Kiemle, *Spectroscopic identification of organic molecules*, 7<sup>th</sup> Edition, John Wiley
6. P. S. Kalsi, *Spectroscopy of Organic Compounds: New Age International Pvt Ltd 6th edition edition,*, 2006

#### REFERENCE:

1. Hollas, J.M., *Modern Spectroscopy*, John Wiley & Sons, Fourth Edition, 2004
2. J. Keeler, *Understanding NMR spectroscopy*, Wiley, 2009
3. D. A. Skoog, F. J. Holler and S. R. Crouch, 'Principles of Instrumental Analysis', 6<sup>th</sup> Edition, Thomson Brooks/Cole, 2007.
4. W. Kemp, *NMR in Chemistry*, McMillan, 1988
5. J. E. Wertz and J. R. Bolton *Electron Spin Resonance*, Springer Science

**Learning Outcomes:** In this course students learn about the basic theories, concepts, instrumentations and specific applications of various spectroscopic techniques in details. This knowledge is essential for the students pursue higher studies in chemistry, to take part in research and development and or to seek a profession related to chemistry.

#### Evaluation Pattern – R.13 & R.16

18CHY513

Organic Reaction Mechanism

3 1 0 4

#### Course Outcomes

The course will help students to

**CO 1:** Understand nucleophile and electrophile groups and their properties.

**CO 2:** Describe and demonstrate the importance of molecular rearrangements in organic compound synthesis and understand the basics of photochemistry and pericyclic reactions.

**CO 3:** Describe the interaction of excited states with their surroundings and analyse photo-induced electron transfer/excitation energy transfer reactions.

#### Course Contents:

**Unit 1** Nucleophilic Substitution: SN1, SN2, and Borderline (ion pair), SNi, SET mechanisms, Neighboring group participation, substitution at allylic carbons, substitution at aliphatic trigonal carbon, substitution at vinylic carbon. Effect of substrate structure, nucleophile, leaving group and medium on reactivity. Ambident nucleophiles and substrates. Aromatic nucleophilic substitution: SNAr, SN1, benzyne and SRN1 mechanisms. Effect of substrate structure, leaving group and attacking nucleophile on reactivity.

**Unit 2** Electrophilic substitution: SE2 and SEi, SE1, substitution accompanied by double bond shift. Effect of substrate, leaving group, and solvent on reactivity. Aromatic electrophilic substitution: Arenium mechanism, Structure – reactivity relationship, substituent effect, o/p ratio, ipso substitution, orientation and reactivity, quantitative treatment.

Free radical reactions: Radical addition. Effect of substrate (aliphatic, aromatic, bridgehead), nature of the radical and solvent on reactivity.

**Unit 3** Addition reactions: Mechanism of Electrophilic, nucleophilic and radical addition. Addition to conjugated systems. Orientation and reactivity. Addition of hydrogen halides, Oxymercuration, halogenation, sulfenylation, selenylation, addition involving epoxides, addition via organoborane. Addition of water, alcohol, sulfides, to aldehydes, ketones, imines, isothiocyanates, nitrocompounds, nitriles. Mannich reaction,

Elimination reactions: Mechanism of elimination reactions E2, E1, E1CB, steric effect. Effect of substrate structure, base, leaving group and medium on reactivity. Mechanism of pyrolytic elimination.

**Unit 4** Rearrangement reaction: Mechanism of Nucleophilic, electrophilic and radical rearrangements. Nature of migration, migratory aptitudes, memory effects. Wagner-Meerwein, Pinacol, Demjanov, dienone-phenol, Benzil-Benzilic acid, Favorskii, Wolff, Neber, Hofmann, Curtius, Lossen, Schmidt, Beckmann, Baeyer-Villiger, Stevens, benzidine, Hofmann-Löffler and Chapman rearrangements and their mechanisms.

**Unit 5** Photochemistry and pericyclic reactions: General principles – Fate of excited state – Jablonsky diagram - chemical process – Photochemistry of alkenes, dienes and polyenes, Carbonyl compounds, Norrish type 1 and Type 2, Paterno–Buchi reaction.

Pericyclic reactions: Cyclo addition - Diels-Alder reaction, Substituent effect on reactivity, regioselectivity and stereochemistry, Catalysis of Lewis acids, Synthetic applications, Enantio selective Diels alder reactions, Intramolecular Diels-Alder reactions. 1,3 Dipolar Cycloaddition – reactivity, regio and stereoselectivity, Applications. [2+2] cycloaddition – ketenes and alkenes – photochemical Electrocyclic reactions, Orbital symmetry, charged species. Sigmatropic rearrangements – [1,3], [1,5], and [1,7] sigmatropic shifts – [3,3] sigmatropic rearrangements – Cope, Oxy-Cope and Claisen rearrangement. [2,3] rearrangements – oxides and ylides – Wittig and aza – Wittig rearrangements, Cheletropic reactions.

#### TEXT BOOKS

1. Michael B Smith, “March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure”, 7<sup>th</sup> edition, Wiley (2015).
2. Francis A.Carey and Richard J. Sundberg, “Advanced Organic Chemistry - Part A: Structure and Mechanisms”, 5<sup>th</sup> Edition, Springer, 2008
3. Francis A.Carey and Richard J. Sundberg, “Advanced Organic Chemistry - Part B: Reactions and Synthesis”, 5<sup>th</sup> Edition, Springer, 2008.
4. Singh S P and SM Mukherji, “Reaction Mechanism in Organic Chemistry”, 2014

#### REFERENCES

1. Reinhard Bruckner, Advanced Organic Chemistry, Reaction Mechanisms, Elsevier, 2002
2. R.O.C. Norman and J.M. Coxon, “Principles of organic synthesis”, CRC press, 2014
3. Ian Fleming, Frontier Orbitals and Organic Chemical Reactions 1st Edition, Wiley, 1991.

**Learning Outcomes:** In this course students learn about the various types of the mechanisms observed in organic transformation reactions, including several named reactions of industrial applications. This knowledge is essential for the students to continue their studies in synthetic chemistry, to take part in research and development and to seek a profession related to synthetic chemistry.

### Evaluation Pattern – R.13 & R.16

18CHY514

Heterocyclic and Natural Product chemistry

3 0 0 3

#### Course Outcomes

After completing the course, the students will be able to

**CO 1:** Explain on mechanistic level, reactions and synthesis of important nitrogen/oxygen/Sulphur containing heterocycles; pyrroles, pyridines, diazoles, diazines, benzo-condensed analogs, furan and

thiophenes

**CO 2:** Understand the fundamentals of carbohydrate chemistry

**CO 3:** Provide an overview of field of biochemistry and natural product chemistry, their occurrence, structure, total synthesis, biosynthesis and properties.

### **Course Contents:**

#### **Unit 1 Heterocyclic compounds**

Nomenclature and general characteristics of heterocyclic compounds, study of three and four-membered ring heterocycles containing one heteroatom, structure and synthesis of penicillin and cephalosporin-C, structure and synthesis of reserpine, heteroaromatic compounds (five and six-membered rings) containing one and two heteroatoms, fused ring compounds - indole, quinoline, isoquinoline, coumarin, flavones, purine and pyrimidine, bases present in nucleosides.

#### **Unit 2 Carbohydrates and nucleic acids**

Nomenclature – aldoses, ketoses, furanoses, pyranoses. Classification – monosaccharides, disaccharides and polysaccharides. Structure (Fischer, Haworth and chair projection) of ribose, glucose, fructose, maltose, sucrose, lactose, starch, cellulose and cyclodextrins. Preparation of alditols, glycosides, deoxysugars. Biosynthesis of vitamin C from glucose. Structure and synthesis of nucleic acids, genetic code, recombinant DNA. biosynthesis of shikimic acid

#### **Unit 3 Chemistry of Natural Products**

Alkaloids - classification, structure elucidation based on degradative reactions (quinine atropine), Terpenoids - classification, structure elucidation and synthesis of abietic acid, terpenoids. Total synthesis of quinine and papavarine (morphine, heroin).

#### **Unit 4 Steroids**

Steroids - classification, structure of cholesterol, conversion of cholesterol to progesterone, androsterone and testosterone, classification, structure and synthesis of prostaglandins, biosynthesis of fatty acids, prostaglandins, and steroids.

#### **Unit 5 Amino acids, Peptides and Enzymes**

Synthesis of amino acids - Strecker and azlactone synthesis, reactions of amino acids, structure of proteins, introduction to enzymes and coenzymes with special reference to the function of chymotrypsin, NAD, thiamine, pyridoxal, solid phase synthesis – choice of resin, classification and reactions leading to peptide formation.

### **TEXT BOOKS**

1. I.L. Finar Organic Chemistry vol 2 ( 3rd.ed.) Longmans Green & Co. 1964
2. Sujata V. Bhat, Bhimsen A. Nagasampagi, Meenakshi Sivakumar, Chemistry of Natural Products, Springer 2005

### **REFERENCES**

1. K. C. Nicolaou, Eric J. Sorensen, Classics in Total synthesis, Wiley, 1996.
2. Ashutosh kar, Chemistry of Natural Products, (Volume I and II), CBS

**Learning Outcomes:** This course gives advanced knowledge on classification, preparation and reactions of polynuclear aromatic compounds, heterocyclic compounds, carbohydrates, amino acids, peptides, nucleic acids and natural products. By learning this course students will be able understand the importance of these compounds in organic, pharmaceutical and biological chemistry.

**Course Outcomes**

After completing the course the students will be gaining

**CO 1:** An understanding of the history and overview on organometallic compounds (nomenclature, hapticity, 18-electron and 16-electron rules).

**CO 2:** An in-depth knowledge on metal carbonyls and their bondings, CVE based structure prediction and their IR spectral features is obtained.

**CO 3:** A great insight in to the organometallic compounds with interesting ligands and their bondings combined with structural features.

**CO 4:** Good knowledge of organometallic compounds with metal carbenes structures (Fischer carbenes, Schrock carbenes and *N*-heterocyclic carbenes, metal polyenes, metal carbines, metal alkyl/aryl derivatives).

**CO 5:** An understanding of the basics of fragment molecular orbitals (FMO) of various organic and inorganic moieties and their symmetry and shapes.

**CO 6:** The ability to predict the iso-electronic and isolobal relationships between various organic and inorganic ( $ML_n$ ) fragments and their MO level diagrams.

**CO 7:** An understanding about stereochemically non-rigid molecules, fluxional nature of organometallic compounds and their characterisation by NMR spectroscopy.

**CO 8:** An insight into the basics of reactions involving various organometallic compounds: oxidative addition reactions, reductive elimination reactions, migratory insertion reactions, 1,1-type and 1,2-type insertion reactions, elimination reactions,  $\beta$ -hydride elimination reactions.

**CO 9:** An in-depth knowledge on the application of basic organometallic reactions into the various types of catalytic processes for the synthesis of various organic compounds is obtained.

**CO 10:** A knowhow of the importance of organometallics in industry, in medicine, in agriculture and in environmental science.

**Course Contents:****Unit 1: Concepts and Metal Carbonyls**

History and overview on organometallic compounds. Classification and nomenclature – hapticity of fragments, 18-electron and 16-electron organometallic compounds. Structure prediction based on '18 electron rule'. Metal carbonyls – synthesis and bonding of metal carbonyls (based on MO theory), donor and acceptor properties of CO, different types of binding modes of CO, poly-nuclear carbonyls with and without bridging groups, metal-metal bonding in M-CO clusters, cluster valence electron (CVE) count, CVE based structure prediction. IR spectral features of metal carbonyls, activation of CO by bonding with metal ions.

**Unit 2: Types of organometallic compounds**

Metal phosphines compounds of transition metals, M-N<sub>2</sub> (metal dioxygen), M-O<sub>2</sub> (metal dioxygen), M-NO (metal nitrosyl) and M-CN (metal cyanide/isocyanide) complexes, bonding and structural features. Organometallic compounds with  $\pi$ -donor ligands like olefins, acetylenes and allyl moieties. Metal derivatives of cyclic  $\pi$ -donors (metallocenes, sandwich/half-sandwich compounds, bent metallocenes), metal-carbon  $\sigma$ -donors (metal carbenes – Fischer carbenes, Schrock carbenes and *N*-heterocyclic carbenes, metal polyenes, metal carbines, metal alkyl/aryl derivatives). Organometallic chemistry of lithium and magnesium, aluminum alkyls and all other main-group organometallics. Structural features and nature of bonding in above compounds.

### Unit 3: Structure and Bonding

Fragment molecular orbitals (FMO) of various organic and inorganic moieties like  $\text{CH}_3$ ,  $\text{CH}_2$ ,  $\text{CH}$ ,  $\text{BH}_2$ ,  $\text{BH}$ ,  $\text{NH}_2$ ,  $\text{NH}$ . FMO's ( $\pi$ -orbitals) of  $\text{C}_3\text{H}_5$ ,  $\text{C}_4\text{H}_4$ ,  $\text{C}_4\text{H}_6$ ,  $\text{C}_5\text{H}_5$ ,  $\text{C}_6\text{H}_6$ ,  $\text{C}_8\text{H}_8$ . Inorganic fragments  $\text{ML}_n$  with varying number of L's. Symmetry and shape of their FMO's. Isolobal concept, iso-electronic and isolobal relationships between various organic and inorganic ( $\text{ML}_n$ ) fragments. Structure and bonding between various organic and inorganic fragments based on MO level diagrams – metal-olefins,  $\text{ML}_n$ -cyclobutadiene,  $\text{ML}_n$ -carbene,  $\text{ML}_n$ -carbyne,  $\text{ML}_n$ -cyclopentadienyl systems, compounds with metal-metal multiple bonds (metal-metal  $\sigma$ ,  $\pi$  and  $\delta$  bonds).

### Unit 4: Stereochemistry and reactions

Stereochemically non-rigid molecules, fluxional nature of organometallic compounds (including Li-C, Mg-C), characterization of non-rigidity of organometallic compounds by NMR spectroscopy. Difference in NMR spectra of fluxional organometallic compounds at high and low temperatures. Characterization techniques of organometallic compounds (by NMR –  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{31}\text{P}$  NMR spectroscopy, Dynamic NMR, Mass spectrometry). Reactions involving various organometallic compounds - oxidative addition reactions, reductive elimination reactions, migratory insertion reactions, 1,1-type and 1,2-type insertion reactions, elimination reactions,  $\beta$ -hydride elimination reactions. Conditions for organometallic compounds to exhibit above reactions, cyclo-metalation and ortho-metalation reactions, agostic interactions.

### Unit 5: Organometallic Catalysis

Alkene hydrogenation using Wilkinson's catalyst, water-gas shift reaction, Mosanto process, Cativa Process. Reaction steps in the above catalytic processes. Hydro-formylation reactions, catalytic addition of molecular oxygen to alkenes (Wacker process), Ziegler-Natta polymerization of alkenes, Fischer-Tropsch process, olefin-metathesis (types of Grubbs catalysts and Hoveyda-Grubbs catalysts), oligomerization of alkynes, aluminum alkyls in polymerization of olefins. Palladium based reactions such as Heck, Stille, Suzuki, Sonogashira, Buchwald-Hartwig couplings; Tsuji-Trost C-C bond formations. Homogeneous vs. heterogeneous organometallic catalysis (principles, mechanism and their applications). Organometallics - in industry, in medicine, in agriculture and in environmental science.

#### TEXTBOOKS:

1. J.E. Huheey, R.A. Keiter, R.L. Keiter, 'Inorganic Chemistry-Principles of Structure and Reactivity', 4<sup>th</sup>Edn., Prentice Hall, 1997.
2. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, 'Shriver and Atkins Inorganic Chemistry', 4<sup>th</sup>Edn., Oxford University Press, 2006.
3. F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, 'Advanced Inorganic Chemistry', 6<sup>th</sup>Edn., Wiley-Interscience, 1999.
4. Anil Elias, Gupta B.D., "Basic Organometallic Chemistry", Universities Press; 2<sup>nd</sup>Edition 2013
5. J.D. Atwood, 'Inorganic and Organometallic Reaction Mechanism', 2<sup>nd</sup>Edn., Wiley-

#### REFERENCES:

1. R. H. Crabtree, 'Organometallic Chemistry of the Transition Metals', John Wiley & Sons, 6<sup>th</sup> Ed.
2. VCH, 1997.
3. J. Tsuji, 'Transition metal reagents and catalyst innovations in organic synthesis', John-Wiley- & Sons, Ltd, New York, 2000
4. B.E. Douglas, D.H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3<sup>rd</sup>Edn., Wiley-India, 2007.
5. M. Bochmann, Organometallics: Complexes with Transition Metal-Carbon Sigma Bonds, Oxford University Press, 1994.
6. J. P. Collman, R G Finke and J R Norton "Principles and Applications of Organo-transition metal Chemistry" University Science Books, 1987.
7. W.K. Li, G.D. Zhou, T. Mak, Advanced Structural Inorganic Chemistry, Oxford University Press, 2008.
8. K. C. Nicolaou, 'Classics in Total Synthesis', Vols I-III, Wiley-VCH, 1996; 2003; 2011

**Learning Outcomes:** In this course students learn about the concepts of organometallic chemistry, theories and concepts, synthesis, bonding, structure, characterizations, functional properties and the applications of coordination compounds in various fields, like, medicine and catalysis. This knowledge is essential for the students to pursue their higher studies in inorganic chemistry, organometallic chemistry or catalysis and to seek a profession related to catalysis or medicinal chemistry.

## Evaluation Pattern – R.13 & R.16

### 18CHY581 INORGANIC SEMI-MICRO QUALITATIVE ANALYSIS LAB. 0 0 6 2

#### Course Outcomes

After the course, the students will be in a position

**CO 1:** To understand the distinction between qualitative and quantitative chemical analyses

**CO 2:** To acquire theoretical knowledge on quantification of an analyte present in a sample through volumetrically and gravimetrically

**CO 3:** To perform volumetric and gravimetric experiments using conventional equipment/apparatus, instrumentation and techniques

**CO 4:** To attain skills in laboratory data collection, formal documentation and interpretation of the collected data

#### Semi micro analysis of mixtures

The mixture will include 4 cations including two common (eg. Cations of metals like Cu, Mn, Zn, Ni, Ca, Ba, Mg etc) and two less common cations (eg. Cations of metals like Ti, Zr, V, W, Li, Ce, Th etc).

*(The student has to successfully analyze a minimum of 10 mixtures).*

#### TEXTBOOKS:

1. A. I. Vogel, 'A text book of Qualitative Analyses', 4<sup>th</sup> edition, Longmans publications, 1985.
2. V.V. Ramanujam, 'Inorganic Semi-Micro Qualitative Analysis', 3<sup>rd</sup> edition, The National Publishing Company, 1974.

#### REFERENCES:

1. G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, 'Vogel's Text Book of Qualitative Chemical Analysis', 5<sup>th</sup> edition, John Wiley & Sons Inc, 1989.
2. G.W. Parshall, 'Inorganic Synthesis', Vol. 15, Tata McGraw-Hill Education, 1974.

**Learning Outcomes:** The methods used in analysing the different inorganic cations and their chemistry. It is very useful in the various applications like food safety and pharmaceuticals.

## Evaluation Pattern – R.13 & R.16

### 18CHY582 ORGANIC QUANTITATIVE ANALYSIS LAB. 0 0 6 2

#### Course Outcomes

After the course, the students will gain

**CO1:** Impeccable understanding to calculate a limiting reagent, yield, and percent yield. Also, ability to



summarize findings in a clear and concise manner

**CO 2:** Knowledge of safe laboratory practices handling laboratory glassware, equipment, and chemical reagents including how to perform common laboratory techniques, including reflux, distillation, steam distillation, recrystallization, vacuum filtration, aqueous extraction, thin layer chromatography, column chromatography.

**CO 3:** Wide knowledge in prediction of outcome and mechanism of some simple organic reactions, using a basic understanding of the relative reactivity of functional groups.

**CO 4:** Basic knowledge in characterizing organic molecules by physical and spectroscopic means, including melting point, boiling point, Infrared red spectroscopy and NMR.

### **Course Contents:**

#### **A. Estimations:**

Estimation of equivalent weight of an acid

Estimation of glucose

Estimation of phenol

Estimation of acetone

Estimation of acid value of an oil

Estimation of iodine value and saponification value of an oil

Estimation of Nitrogen – Kjeldahl method

Estimation of formaldehyde

Estimation of aniline

Estimation of ester

#### **B. Preparations of Organic Compounds**

Double stage preparations

(a) m-nitro benzoic acid from ethyl benzoate

(b) p-bromobenzanilide from aniline

(c) p-nitro acetanilide from aniline

Single stage preparations

(a) Benzimidazole

(b) Benzophenone oxime

(c) Dibenzilidene acetone (chalcone)

(d) Benzalacetophenone

(e) Benzanilide

(f) Acetanilide

(g) Acetyl salicylic acid (aspirin)

Name Reactions

(a) Benzil-Benzilic acid rearrangement

(b) Cannizzaro reaction

(c) Claisen condensation

For all preparations

1. TLC to be done and R<sub>f</sub> values of each compound to be reported
2. Melting point of pure compounds to be found
3. A small portion should be recrystallised from suitable solvent
4. Purified products to be displayed
5. Mechanisms for each preparation should be suggested

## REFERENCES:

1. P.W.G. Smith, A.J.Hannaford, B.S.Furnis and A.R. Tatchell, "Vogel's Textbook of Practical Organic Chemistry", ELBS/Logman, 1989.
2. Ralph L. Shriner, Christine K. F. Hermann, Terence C. Morrill, David Y. Curtin, Reynold C. Fuson, 'Systematic Identification of Organic Compounds', John Wiley & Sons, 2003.
3. Mann and Saunders, 'Practical Organic Chemistry', Pearson edition, 2009.

**Learning Outcomes:** In this course students get the training on synthesis, extraction, purification and characterization of some important organic compounds. They also perform some named reactions of synthetic importance. Students also get the information about elemental estimation techniques. This knowledge is essential for the students to continue their studies in synthetic chemistry, to take part in research and development and to seek a profession related to synthetic chemistry.

## Evaluation Pattern – R.13 & R.16

**18CHY583      ADVANCED PHYSICAL CHEMISTRY LAB.**

**0 0 5 2**

### Course Outcomes

After the course, students will gain

**CO 1:** Skill to evaluate the kinetics of different chemical reactions and to determine the activation energy for reactions.

**CO 2:** Ability to analyse the thermodynamic parameters in phase equilibrium

**CO 3:** Knowledge of optical properties of materials and apply this for analytical applications

**CO 4:** Knowledge to create experiments to evaluate physical chemistry concepts

### Course Contents:

1. Construction of phase diagram for three component system.
2. Determination of equivalent conductance at infinite dilution of weak electrolytes.
3. Determination of order of reaction for ion exchange reaction.
4. Extraction efficiency of solute from a solution by immiscible solvent method.
5. Determination of calorific value using Bomb calorimeter.
6. Kinematic viscosity of lubricants using Bomb calorimeter.
7. Determination of the formation constant of silver-ammonia complex and stoichiometry of the complex potentiometrically.
8. Determination of flash point, fire point of a lubricant.
9. Determination of cloud point and pour point of a lubricant.

### TEXTBOOKS:

1. Alexander Findly, 'Practical physical chemistry', 9<sup>th</sup> edition, Wiley, 1972.
2. R.C.Das and B.Behera, 'Experimental Physical Chemistry', Tata McGraw-Hill, 1983.

### REFERENCE BOOKS:

1. J.B.Yadav, 'Advanced Practical Physical Chemistry', Krishna Prakashan Media, 29<sup>th</sup> edition, 2010.
2. Francis William Gray, 'A Manual of Practical Physical Chemistry' Macmillan and Co., Limited, 1914.

**Learning Outcomes:** In this course students get the training on advanced techniques and methods used in the determination of various parameters of chemical compounds and their reactions. This knowledge is essential for the students to continue their studies in chemistry, to take part in research and development and

to seek a profession related to analytical and industrial chemistry.

## Evaluation Pattern – R.13 & R.16

**18CHY584 INORGANIC QUANTITATIVE ANALYSIS LAB. 0 0 6 2**

### Course Outcomes

This course will help students

**CO 1:** To understand the distinction between qualitative and quantitative chemical analyses

**CO 2:** To acquire theoretical knowledge on quantification of an analyte present in a sample through volumetrically and gravimetrically

**CO 3:** To perform volumetric and gravimetric experiments using conventional equipment/apparatus, instrumentation and techniques

**CO 4:** To attain skills in laboratory data collection, formal documentation and interpretation of the collected data

### Course Contents:

1. Estimation of Calcium (Permanganometry)
2. Estimation of Barium (Iodometry)
3. Estimation of Calcium as Calcium Carbonate (Gravimetry)
4. Estimation of Zinc using oxine (Gravimetry)
5. Estimation of Iron as Ferric Oxide (Gravimetry)
6. Analysis of Brass
7. Estimation of Copper and Nickel in a Mixture
8. Estimation of Copper and Iron in a Mixture
9. Preparation and Determination of Ferrous Oxalate
10. Estimation of Different Types of Hardness in the Given Water Sample
11. Estimation of Different Types of Alkalinities in the Given Water Sample
12. Estimation of Dissolved Oxygen in the Given Water Sample
13. Complexometric Estimations

### TEXTBOOKS:

1. G. Svehla, 'Vogel's Qualitative Inorganic Analysis', 7<sup>th</sup> Edition, Prentice Hall, 1996.
2. D. A. Skoog and D. M. West, 'Analytical Chemistry - An Introduction', 4<sup>th</sup> Edition, CBS Publishing Japan Ltd., 1986.

### REFERENCES

1. E.J.Meehan, S.Bruckenstein and I.M.Kolthoff and E.B.Sandell, 'Quantitative Chemical Analysis', 4<sup>th</sup> Edition, The Macmillan Company, 1969.
2. R.A.Day (Jr) and A.L.Underwood, 'Quantitative Analysis', 6<sup>th</sup> Edition, Prentice Hall of India, 1991.

**Learning Outcomes:** In this course students get the training of various methods used in the quantitative estimation several metal ions or mixture of metal ions. They also learn the methods for estimation of hardness, alkalinity and dissolved oxygen of water. This knowledge is essential for the students to continue their studies in chemistry, to take part in research and development and to seek a profession related to analytical and environmental chemistry.

## Evaluation Pattern – R.13 & R.16

**Course Outcomes**

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

**CO 1:** Compute physical quantities based on equations

**CO 2:** Analyse the behaviour of solutions of electrolytes

**CO 3:** Deduce the mechanism of chemical reactions

**CO 4:** Deduce the kinetics of chemical reactions

**CO 5:** Have a thorough knowledge about the laws and theory

**CO 6:** Understand the applications of the laws and theory

**CO 7:** Predict and understand about the mechanism

**CO 8:** Gain knowledge about the instruments used for various analytical work

**CO 9:** Gain knowledge on batteries and fuel cells

**Course Contents:****Unit 1 Surface Chemistry**

Different types of interfaces, molecular and atomic surface structure, surface chemical reactions, surface tension of solutions, surface excess, thermodynamics of surfaces, Gibbs equation and its derivation, surface films, surface potential, adsorption by solids, Langmuir isotherm - its kinetic and statistical derivation, Freundlich equation, multilayer adsorption, BET isotherm - its kinetic derivation, measurement of surface area.

Colloids - their preparation, purification, stability & electro kinetic phenomena, Donnan membrane equilibrium, micro and nano emulsions.

Surface analysis using photoelectron spectroscopy, surface imaging techniques like SEM, TEM, AFM etc., sputter coating, ion beam principles, design of surfaces with novel properties.

**Unit 2 Electrochemistry I**

Review of Faraday's laws, conductivity of electrolytes, ionic mobility, transference number, Kohlrausch law, pH of acids, bases and buffers, solubility product and salt hydrolysis and Ostwald dilution law. Deviations from the Ostwald law, activity and activity coefficients in electrolytic solution, Modern theory of conductance of strong electrolytes and its tests and improvements, Debye-Huckel-Onsager equation – theory of mean activity coefficients of strong electrolyte – Debye-Huckel Limiting Law and its testing and improvement.

**Unit 3 Electrochemistry II**

Electrochemical cells, standard electrode potentials, reversible cell, concentration cells with and without transference, standard electrode potentials, reversible cell, cell notation and calculation of emf – variation of potential with concentration, pressure and temperature, Liquid Junction Potential – its calculation and elimination - Thermodynamics of cell reactions and equilibrium constant - applications of e.m.f. measurements, potentiometric measurement of pH –reference electrodes - glass and quin-hydrone electrodes and their performance and limitations, – ion selective electrodes – biomembranes, Interfacial region – electrical double layers and their structure – Helmholtz-Perrin, Gouy-Chapman and Stern models - charge transfer across interfaces, mass transport – diffusion and convection controlled transport – irreversible electrode processes - activation, concentration and IR polarisation, decomposition potential, Butler-Vohmer equation - over potential (hydrogen, oxygen and metal decomposition over voltage), theories of over voltage, Tafel equation, and Tafel plots – corrosion and its rate from Tafel equation.

**Unit 4 Chemical Kinetics I**

Reaction rates and order of reactions, determination of order of reactions, complex reactions, reversible, consecutive and concurrent reactions, reactions of variable order, steady state treatment, reaction mechanism and molecularity, theories of unimolecular reactions and termolecular reactions, Arrhenius equation, collision theory and transition state theory, comparative study of the theories of reaction rates, free energy of activation, effect of solvent on rate of reactions, ionic reactions and effect of ionic strength - salt effect, effect of pressure on velocity of gas reactions.

### Unit 5 Chemical Kinetics II

Reaction dynamics, fast reactions, flash photolysis and relaxation methods, catalysis and inhibition, homogeneous catalysis, acid, base and enzyme catalysis, kinetics of enzyme catalyzed reaction - the Michaelis-Menten equation. Photochemical kinetics, steady state treatment of photochemical reactions, Semenov-Hinshelwood theory of chain reactions and explosions, free radical reactions - the Rice-Herzfeld mechanism.

#### TEXTBOOKS:

1. Gilbert W. Castellan, "Physical Chemistry", 3<sup>rd</sup> Edition, Narosa Publishing House, 2004.
2. K. J. Laidler, 'Chemical-Kinetics', 3<sup>rd</sup> Edition, McGraw Hill, New York, 2004.
3. An introduction to Electrochemistry, Samuel Glassstone (2007)

#### REFERENCES:

1. W. J. Moore and R. G. Pearson, 'Kinetics and Mechanism', 2<sup>nd</sup> edition, Wiley, 1981.
2. Physical Chemistry, Peter Atkins, Julio D Paula, OUP Oxford; 9 edition (19 November (2009)
3. Textbook of Physical Chemistry, Samuel Glassstone, D. Van Nostrand company, inc; 2nd edition (1946)
4. John O'M. Bockris, Amulya K.N. Reddy, Modern Electrochemistry 1: Ionics, 2<sup>nd</sup> Edition, Springer, 1998
5. John O'M. Bockris, Amulya K.N. Reddy, Maria E. Gamboa-Aldeco, Modern Electrochemistry 2A: Fundamentals of Electrochemistry 2nd Edition, Springer, 2001

**Learning Outcomes:** This course gives detailed basic and concise advanced knowledge of the fields, Surface chemistry, chemical kinetics and electrochemistry, which is essential for the better understanding of chemistry and advancement.

## Evaluation Pattern – R.13 & R.16

18CHY602

Synthetic Strategies and Reagents

3 1 0 4

### Course Outcomes

After the completion of the course the students will have an understanding of

**CO 1:** Pericyclic reactions, principle of conservation of orbital symmetry, thermal and photochemical reactions, selection rules, electrocyclic reactions, cycloadditions, sigmatropic rearrangements

**CO 2:** Retrosynthetic analysis-ways to synthesize organic molecules from simple starting materials

**CO 3:** Organometallic reagents, methods of preparing them and the reactions carried out using them

**CO 4:** Various oxidation and reduction reactions and the reagents that are used for such reactions.

**CO 5:** Base catalyzed reactions and an in-depth knowledge on various name reactions using different type of bases.

### Course Contents:

#### Unit 1 Synthetic Strategies

Synthetic strategies: Functional group inter-conversion – conversion of one functional group to other. Nitrogen, oxygen, sulphur protection and deprotection – utilization of protection groups in organic synthesis. Retro synthetic analysis, functional group equivalents, use of retrosynthesis in organic synthesis.

Reversal of reactivity (Umpolung), Introduction to combinatorial chemistry. Application of phase transfer catalysts.

### **Unit 2 Oxidation and reduction:**

PCC, DDQ, DMSO, Dess-Martin Reagent, TEMPO, osmium tetroxide, ruthenium tetroxide, selenium dioxide, peracids, hydrogen peroxide, singlet oxygen, aluminum isopropoxide, periodic acid, lead tetraacetate. Swern, Jones, Oppenauer oxidation, Woodward and Prevost hydroxylation, Sharpless asymmetric epoxidation, catalytic hydrogenations (heterogeneous and homogeneous), Clemmensen, Wolff Kishner, Rosenmund and MPV reductions, metal hydrides as reagents (aluminium/boron hydrides and hydroboration reaction), Birch reduction, Borche Reduction, hydrazine and diimide reduction.

**Unit 3 Organometallic reagents:** Preparation, properties and reactions of organo lithium, organosilicon, organozinc (Reformatsky reaction) and organomagnesium reagents (Barbier and Grignard), organocadmium, organo mercury reagents based organometallic reactions involving C-C bond formation. Selected functional group transformations in organic synthesis. Preparation and reactions of Organo copper, organopalladium,- Wacker process – Heck reaction, cross coupling, carbonylation reaction, organonickel, organo cobalt and organo rhodium reagents – Olefin metathesis reaction. Reactions and applications of Organoboron, organo silicon and organotin compounds.

### **Unit 4 C-C, bond formation**

C-C bond formation – aldol, Arndt-Eistert, Bardhan-Sengupta, Baker-Venkataraman, Barbier, Baylis-Hillman, Benzoin, Heck, Fukuyama, Dieckmann, Friedel-Crafts, Michael, Perkin, Claisen, Robinson annulations, Vilsmeier, Wittig, Knoevnagel, Michael additions.

### **Unit 5 C-N, C-O bond formations**

C-O bond formation – barton, Fischer esterification, Prins, Darzen, Baeyer-Villiger, Mitsunobu, Williamson's ether synthesis, Ullman Coupling with Boronic Acids.

C-N bond formation – Mannich, Fukuyama, Mitsunobu, Ritter, Gabriel Synthesis, Ugi, Doebner Reaction, Buchwald-Hartwig, Stork-enamine, formation of azides and hydrazines, formation of amides and peptides, coupling reactions.

### **TEXT BOOKS**

1. Modern Organic Synthesis, Dale L. Boger, The Scripps Research Institute, Rush Press, San Diego, California, 2001
2. Francis A. Carey and Richard J. Sundberg, "Advanced Organic Chemistry - Part B: Reactions and Synthesis", 5<sup>th</sup> Edition, Springer, 2008.
3. R.O.C. Norman and J.M. Coxon, "Principles of organic synthesis", CRC press, 2014

### **REFERENCES**

1. Stuart Ware, Designing Organic Synthesis: A programmed introduction to the synthon approach, JOHN WILEY & SONS, 2nd edition, 2008
2. Name Reactions: A collection of detailed Mechanisms and synthetic applications, Jie Jack Li, Springer, fourth edition (expanded edition), 2009.
3. Michael B Smith, "March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure", 7<sup>th</sup> edition, Wiley (2015).
4. Francis A. Carey and Richard J. Sundberg, "Advanced Organic Chemistry - Part A: Structure and Mechanisms", 5<sup>th</sup> Edition, Springer, 2008

**Learning Outcomes:** This course gives advanced knowledge about the various synthetic strategies, importance of redox-steps, C-C, C-N and C-O bond formation and usage of organometallic reagents. This knowledge is essential for the students to continue their studies in synthetic chemistry and catalysis to take part in research and development and to seek a profession in polymer, pharmaceutical or other related industries.

### **Evaluation Pattern – R.13 & R.16**

After completing the course a student will have

**CO 1:** In-depth understanding of the fundamental concepts of crystallographic systems and their symmetries.

**CO 2:** Ability to comprehend the different types of solid structures: Ionic solids, spinels, rutile, fluorite, etc.

**CO 3:** Ability to understand the basics of bonding in different types of solids and their theories.

**CO 4:** In-depth understanding of Band theory and its application in explaining the properties of solids (photoconductivity, electrical conductivity, etc.)

**CO 5:** An understanding of the basics of magnetic properties (ferro and anti-ferro magnetic, super exchange) of solid materials.

**CO 6:** Thorough understanding of the contribution of crystal defects in to various properties of solids: Schottky defects, Frenkel defects, doping in crystals and colour features, ruby, diamond.

**CO 7:** Knowledge of the importance of solid materials and their structure property relationships: Band-gap properties of semiconductors; photo-catalytic properties of ZnO and TiO<sub>2</sub>; inorganic-organic hybrid materials; high T<sub>c</sub> superconductors.

**CO 8:** Knowledge about metal-organic framework (MOF) materials and their special features (gas storage, emission properties and sensors).

**CO 9:** Deep understanding about sol-gel processes, characterization of processed materials by PXRD, IR, Raman, UV-visible and solid state NMR spectral techniques, understanding morphological features through, SEM, EDAX and TEM methods.

**CO 10:** An understanding of chemical vapour deposition (CVD) method for solid state synthesis and synthesis of inorganic-organic hybrid materials; solvo-thermal and high pressure synthesis.

## **Course Contents:**

### **Unit 1 Introduction to Crystal Systems**

Introduction to solids - solid state chemistry, close packing, hcp, fcc, density, coordination numbers, tetrahedral and octahedral holes, body centered and primitive structures, symmetry, proper rotation, mirror planes, inversion, improper axis symmetry elements, symmetry in crystals, Schoenflies and Hermann-Mauguin notations, unit cells, glide plane, screw axis, atom occupancy in cubic unit cells, seven crystal systems/classes, space groups, Miller indices, Bravais lattices, reciprocal lattice, inter-planar spacing in different crystal systems, fractional coordinates, ionic solids, structures of CsCl, NaCl, NiAs, zinc blende and wurtzite structures, MX<sub>2</sub> type solids, fluorite and antiferite structures, CdCl<sub>2</sub> and CdI<sub>2</sub> structures, rutile and anti-rutile, ReO<sub>3</sub>, spinel and inverse spinel, perovskite structures, ionic radii, crystal radii, radius ratio, Extended covalent array, diamond, graphite.

### **Unit 2 Bonding in Solids and Electronic properties**

Bonding in crystals, metallic bonding, ionic bonding, covalent bonding, silicates, Born-Haber cycle, Hess's law, lattice energy (L) and calculation of L, free electron theory, density of states, electronic conductivity, molecular orbital theory, overlap and bonding, linear chain of H atoms, LCAO, Fermi Level, conductors, insulators and semiconductors, n- and p-type semiconductors, bands in compounds, band-gap energy, direct and indirect band gaps in semiconductors, band-gap measurements, electrical conductivity, photo-conductivity.

### **Unit 3 Magnetic and Optical Properties of Solids**

Behaviour of substances in magnetic field, magnetic moments, para magnetism, diamagnetism, ferro- and anti-ferromagnetism, ferri-magnetism, effects of temperature of magnetism, Curie & Curie-Weiss laws; mechanism of ferro- and anti-ferromagnetic ordering, super exchange. Luminescence and phosphorescence of solid materials, phosphors, lasers, non-stoichiometry and its effect in properties of solids, electronic properties of non-stoichiometric oxides. Defects in solids, Schottky defects, Frenkel defects, doping in crystals and colour features, ruby, diamond, organic conductors, preparation, mechanism of conduction in organic semiconductors, photoconductivity of polymers.

### **Unit 4 Materials Science-Structure and properties**

Solid materials of importance. Structure and properties of SiO<sub>2</sub>, ZrO<sub>2</sub>, SiC, BN, ZnO, TiO<sub>2</sub>, CdS, CdTe, GaAs, MoS<sub>2</sub>. Band-gap properties of semiconductors like ZnO, TiO<sub>2</sub>, CdS, CdSe, CdTe, GaAs, MoS<sub>2</sub> and (CH<sub>3</sub>NH<sub>3</sub>)[PbX<sub>3</sub>]-type perovskites. Photo-catalytic properties of ZnO and TiO<sub>2</sub> – principle and applications. Inorganic-organic hybrid materials. High T<sub>c</sub> superconductors (HTS) like Bi-Sr-Ca-Cu oxide based HTS (BSCCO) and Y-Ba-Cu-oxide (YBCO), their structure and properties. Metal-organic framework (MOF) materials, special features of MOF materials. Synthesis, special features and properties of MOF materials like HKUST-1 and MOF-8. Gas storage and emission properties of MOF materials. MOFs as sensors. Zeolites, their special features and properties.

### Unit 5 Materials Science-Synthesis, processing and characterization

Sol and gel, their properties, xerogels. Sol-gel synthesis - synthesis of SiO<sub>2</sub> and TiO<sub>2</sub> through sol-gel process. Calcination and sintering. Characterization of processed materials, PXRD, IR, Raman, UV-visible and solid-state NMR spectral techniques. Understanding morphological features through, SEM, EDAX and TEM methods. Chemical vapour deposition (CVD) method. Solid state synthesis, synthesis of High T<sub>c</sub> superconducting materials like YBCO and BSCCO. Synthesis of inorganic-organic hybrid materials. Solvo-thermal and high-pressure synthesis.

#### TEXTBOOKS:

1. L V Azroff, 'Introduction to Solids', Tata McGraw-Hill publishing company
2. L. E. Smart and E. A. Moore, Solid State Chemistry – An Introduction, 4<sup>th</sup> Edition, CRC Press, 2016.
3. A. R. West, Solid State Chemistry and its Applications, Wiley, 2014
4. C N R Rao, K Biswas, Essentials of Inorganic Materials Synthesis, John Wiley, 2014
5. C N R Rao Chemical Approaches to Synthesis of Materials, Wiley, 1994

#### REFERENCES

1. D. Jiles, "Magnetism and Magnetic Materials", Chapman and Hall, London, 1991.
2. R. E. Hummel, "Electronic Properties of Materials", 3rd ed., Springer-Verlag, New York, 2001.
3. Schubert, U. and Hüsing, N, Synthesis of Inorganic Materials, 3rd edn, VCH-Wiley Verlag GmbH, Weinheim, 2012
4. W.D. Kingery, H.K. Dowe and R.D. Uhlman, Introduction to Ceramics, John Wiley.
5. F.H. Norton, Elements of Ceramics,.
6. M.W. Barsoum, Fundamentals of Ceramics, McGraw Hill.
7. Material Science and Engineering, S.K. Hajra Choudhury, Indian Book Dist.
8. B D Fahlman, Materials Chemistry, 2<sup>nd</sup> Edition, Springer, 2011
9. Stefan Kaskel, The Chemistry of Metal–Organic Frameworks: Synthesis, Characterization, and Applications, Wiley-VCH Verlag GmbH, 2016

**Learning Outcomes:** This course gives advanced knowledge about the solid materials, bonding and structure, electronic, optical and magnetic properties and their applications in various fields. This knowledge is essential for the students to continue their studies in chemistry, material science and catalysis to take part in research and development and to seek a profession in polymer, fuel, paint or other related industries.

### Evaluation Pattern – R.13 & R.16

18CHY604

Bioinorganic Chemistry

3 0 0 3

#### Course Outcomes

After completion of the course a student will

**CO 1:** Understand the basics of metal ions in biology (including photosynthesis, PS-I and PS-II) and electron transport systems in biology.

**CO 2:** Gain knowledge on reactive oxygen species (ROS) and role of antioxidants in biology.



**CO 3:** Understand the theory and mechanistic action of hemoglobin and myoglobin and their model compounds; structure and functions of haemerythrin (Hr) and haemocyanin (Hc).

**CO 4:** Gain knowledge about different types of cytochromes and their role in biology; Fe-S and other non-heme iron proteins.

**CO 5:** Understand the structural basics of metallo-enzymes such as catalases, peroxidases, copper enzymes, superoxide dismutase (SOD), Zn-containing enzymes, nitrogenase enzyme.

**CO 6:** Master the structures of Fe-S clusters, Fe-protein structure, Mo-Fe protein structure, P-cluster and M-centre and their model compounds.

**CO 7:** Understand about role of Zn, Ca, Mn, Ni, Mo and Cr in biological systems and metal toxicity.

**CO 8:** Understand in depth about the basics of metal ion based (Pt, V, Au) drugs, anticancer agents, DNA intercalators, MRI imaging and contrast agents.

**CO 9:** Have knowledge on biomimetic compounds of Fe(II), Co(II) and Cu(II) for Mb and Hc.

**CO 10:** Understand photodynamic therapy (PDT), principles and applications; natural and synthetic ionophores, crown ethers, cryptands and cryptates, calixarenes, cyclo-dextrins and their special properties.

## **Course Contents:**

### **Unit 1: Basics in bio-inorganic chemistry**

Essential elements in biological systems, transport of ions across biological membranes, active and passive transport, metal transport and metallochaperons, Na<sup>+</sup>/K<sup>+</sup> pump and active transport. Metal complexation with biological molecules. Electron transport in biology, electron transport chain (ETC), role of ETC in biological systems. Amino acids, peptides and proteins, primary and secondary structure of proteins,  $\alpha$ -helix and  $\beta$ -sheets forms of proteins and their special features; tertiary and quaternary structures of proteins the type of molecular interactions involved in them. Reactive oxygen species (ROS), generation and function of organic free radicals, action of ROS in biological systems, oxidative stress, antioxidants. Photosynthesis, PS-I and PS-II.

### **Unit 2: Oxygen take-up, transport and storage proteins**

Porphine, corrin, corrole, chlorin and bacteriochlorin. Myoglobin (Mb) and hemoglobin (Hb), their prosthetic groups and functions, mechanism for reversible binding of O<sub>2</sub> in Mb and Hb. Cooperative effect in Hb and its consequence. Behaviour of bound O<sub>2</sub> to Fe(II). Difference between O<sub>2</sub> and CO binding to Hb and Mb, CN<sup>-</sup> poisoning. Structure and functions of haemerythrin (Hr) and haemocyanin (Hc), O<sub>2</sub> binding nature in Hr and Hc, electron transfer processes in them. Cytochromes and their role in biology, cytochrome P-450, cytochrome C-oxidase and oxygen transfer from O<sub>2</sub> to non-activated substrates, monooxygenases, methane monooxygenase (MMO). Fe-S and other non-heme iron proteins, ferredoxins-their structure and special properties, transferrin, ferritin, siderophores, enterobactin, uptake, transport and storage of iron. Sick-cell anemia.

### **Unit 3: Metallo-enzymes**

Catalases – structure and properties reaction mechanism. Peroxidases- glutathione peroxidase, HRP, structure and properties and enzyme reaction mechanism. Cytochrome c peroxidase and lignin peroxidase. Copper enzymes-structure and function, azurin, plastocyanin. Type I, II and III copper proteins. Superoxide dismutase (SOD) - structure and enzymatic reaction mechanisms. Tyrosinase, reaction mechanism. Zn-containing enzymes, carbonic anhydrase and carboxy-peptidases-structure and enzymatic reactions. N<sub>2</sub> fixation, nitrogenase enzyme, Fe-S clusters, Fe-protein structure, Mo-Fe protein structure, P-cluster and M-centre, their model compounds.

### **Unit 4: Other functional roles of metal ions**

Zn in biological systems, Zn-finger proteins – structural features and properties, classifications and their roles in biological systems. Ca<sup>2+</sup> binding proteins, calmodulins. Metal ion based (Pt, V, Au) drugs,

anticancer agents. Cis-platin and its properties. Chelation therapy, macrocyclic antibiotics. Role of Mn, Ni, Mo and Cr in biological systems, metal toxicity and homeostasis, therapeutic complexes. Diseases caused by both excess and deficiency of metal ions, thalassaemia, Wilson disease. DNA intercalators, diagnostic agents, MRI imaging and contrast agents, the role of  $Gd^{3+}$  and other metal ions as contrast agents.

### Unit 5: Biomimetic compounds, metals in medicine

Porphyrins ( $H_2P$ ) and metalloporphyrins (MP), spectral, fluorescence and redox properties of  $H_2P$  and MP. Biomimetic compounds. Fe(II), Co(II) and Cu(II) based model compounds model compounds of Mb and Hc – ‘picket-fence’ porphyrin and its special features. Photodynamic therapy (PDT), principles and applications. Natural and synthetic ionophores, crown ethers, interaction and uptake of alkali metal and alkaline earth metal ions with crown ethers, cryptands and cryptates, calixarenes and their special properties, cyclo-dextrins and their special properties.

#### TEXTBOOKS:

1. J.E. Huheey, R.A. Keiter, R.L. Keiter, Inorganic Chemistry-Principles of Structure and Reactivity, 4<sup>th</sup> Edn., Prentice Hall, 1997.
2. F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6<sup>th</sup> Edn., Wiley-Interscience, 1999.
3. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, Shriver and Atkins Inorganic Chemistry, 4<sup>th</sup> Edn., Oxford University Press, 2006.

#### REFERENCES

1. S. J. Lippard, J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, 1994.
2. J. D. Atwood, Inorganic and Organometallic Reaction Mechanism, 2<sup>nd</sup> Edn., Wiley-VCH, 1997.
3. B.E. Douglas, D.H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3<sup>rd</sup> Edn., Wiley-India, 2007.
4. W. Kaim, B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley & Sons, 1994.
5. M. N. Hughes, The Inorganic Chemistry in Biological Processes, Wiley (1981)

**Learning Outcomes:** In this course students get the detailed knowledge about the concepts of bioinorganic chemistry. Structure and activity profiles of various biomolecules will be familiarized. This course provides all the essential knowledge needed for the students to pursue higher studies, research activities or jobs related to bioinorganic chemistry and pharma.

### Evaluation Pattern – R.13 & R.16

18CHY631

Applied Electrochemistry

3 0 0 3

#### Course Outcomes

The course is intended

**CO 1:** To make students familiar with basic notions of electrochemistry: oxidation-reduction, potential, overvoltage.

**CO 2:** To give students an understanding of the electric double layer theory.

**CO 3:** To ensure that students know fundamental principles of Faraday’s law and able to use it for engineering calculations

**CO 4:** to describe and understand the operation of electrochemical systems for the production of electric energy, i.e. batteries and fuel cells.

**CO 5:** provide students with, both an understanding of the basic concepts of biosensing technology, and an appreciation of the state of the art and future directions.

## Course Contents:

**Unit 1 – Electrode kinetics:** Electron transfer under an interfacial electric field, A two way traffic across the interface: equilibrium and exchange current density. Dependence of the electrochemical reaction rate on over potential-Quantitative version of the Butler Volmer equation. Electrode kinetics involving the semiconductor/solution interface. Techniques of electrode kinetics-preparation of electrode surface. Microelectrodes-applications.

**Unit 2: Industrial Cathodic process** - Electrodeposition of copper, nickel and chromium over mild steel – zinc plating on MS – decorative plating of silver and cold – nano plating and microstructure of deposits - Tests for adhesion, hardness, thickness, uniformity and corrosion resistance of the electro deposits-post plating passivation processes-barrel plating of small components - Electroless deposition of nickel, copper, gold on metal components – making of waveguides and plated through hole boards.

**Unit 3: Industrial Anodic Processes:** Anodising of aluminium and its alloys – baths used, operating conditions and sequence determination of thickness – industrial applications- nano anodizing of titanium, and tantalum – application to sensor field

Electropolishing of ferrous and non-ferrous metals and alloys - mechanism of electropolishing – Electrochemical etching of ferrous and non-ferrous metals –

Special processes: Electrolysis of water – electrowinning of aluminium and sodium – electrolysis of brine-photoelectrochemistry

**Unit4 - Electrochemical energy systems:** Primary batteries: Zinc-carbon (Leclanche type), zinc alkaline (Duracell),; lithium primary cells - liquid cathode, solid cathode and lithium-ferrous sulphide cells Secondary batteries: Lead acid and VRLA (valve regulated (sealed) lead acid), nickel-cadmium, nickel-zinc, nickel-metal hydride batteries, lithium ion batteries, ultra thin lithium polymer cells (comparative account) Advanced Batteries for electric vehicles, requirements of the battery - sodium-beta and redox batteries. Reserve batteries thermally activated batteries - remote activation - pyrotechnic materials: Fuel Cells: Principle, proton exchange membrane (PEM), direct methanol(DMFC), molten carbonate electrolyte (MCFC) fuel cells and outline of biochemical fuel cells.

**Unit5 - Electro chemical sensors:** Potentiometric sensors, solid state Potentiometric chemical sensors, polymeric membrane sensors, ion selective field effect transistor, application, Hydrovolumetric technique-hydrodynamic voltammetric-application, voltammetric sensors-electrode modification application, optical sensors, bioamperometric titration. Methods involving forced convection-hydrodynamic methods.

## Text books

1. Allen J. Bard and Larry R. Faulkner, 'Text book for Electrochemical Methods', 2nd edition, Wiley, 2000.
2. Derek Pletcher and Frank C. Walsh, 'Industrial Electrochemistry', Blackie Academic and Professional, (1993).

## References

1. Christopher M A, Brett, 'Electrochemistry – Principles, Methods and Applications', Oxford University, (2004).
2. Watanabe T, 'Nano-plating: microstructure control theory of plated film and data base of plated film microstructure', Elsevier, Oxford, UK (2004).
3. Kanani N, 'Electroplating and electroless plating of copper and its alloy', ASM International, Metals Park, OH and Metal Finishing Publications, Stevenage, UK (2003).
4. Curtis, 'Electroforming', London, (2004).
5. Rumyantsev E and Davydov A, 'Electrochemical machining of metals', Mir, Moscow, (1989).
6. Peter G Sheasby 'Basics of aluminium anodising', Banbury, Oxon (2001)
7. Robert Brugger 'Nickel Plating' Robert Draper Ltd, Teddington, (1970)
8. J. K. Dennis, T. E. Such, 'Nickel and Chromium Plating, Third Edition' Woodhead

**Learning Outcomes:** This course enables the students to understand principles and applications of electrochemical processes, industrial cathodic and anodic processes, electrochemical energy systems (batteries) and electrochemical sensors. This knowledge will enable them to seek advanced courses and professions related to battery technology and energy.

## **Evaluation Pattern – R.13 & R.16**

**18CHY632**

**BIOANALYTICAL CHEMISTRY**

**3 0 0 3**

### **Course Contents:**

#### **Unit 1 Enzymes**

Enzyme nomenclature, Enzyme commission numbers, Enzymes in bioanalytical chemistry, Enzyme kinetics - Enzyme activators, Enzyme inhibitors.

#### **Unit 2 Quantification of Enzymes and their substrates**

Instrumental methods, Optical detection - Absorbance, Fluorescence, Luminescence, Nephelometry  
Electrochemical detection -Amperometry, Potentiometry, Conductometry, Other Detection Methods -  
Radiochemical, Manometry, Calorimetry.

#### **Unit 3 Immobilized enzymes**

Immobilization methods - nanopolymerizing covalent immobilization, Crosslinking with bifunctional reagents. Properties of immobilized enzymes, immobilized enzyme reactions, theoretical treatment of packed bed enzyme reactors.

#### **Unit 4 Antibodies**

Structural and functional properties of antibodies, Polyclonal and monoclonal antibodies Antibody-antigen interactions, analytical application of secondary antibody-antigen.

#### **Unit 5 Biosensors**

Response of Enzyme-based Biosensors, Examples of Biosensor Configuration, Ferrocene-mediated Amperometric Glucose Sensor, Potentiometric Biosensor for Phenyl Acetate, Potentiometric Immunosensor for Digoxin, Optical Biosensor for Glucose Based on Fluorescence Energy Transfer, Piezoelectric Sensor for Nucleic Acid Detection, Enzyme Thermistors.

#### **TEXTBOOKS:**

1. Susan R. Mikkelsen, and Eduardo Corto'n 'Bioanalytical Chemistry', 1<sup>st</sup> edition, Wiley Interscience, 2003.
2. Andres Manz, Nicole Pamme and Dimitri Lossifidis, 'Bioanalytical Chemistry', World Scientific Publishing Company, 2004.

#### **REFERENCE:**

1. Robert W. Cattrall, 'Chemical Sensors', Oxford University Press, 1997.

**Learning Outcomes:** This course provides the detailed information about the qualitative and quantitative analysis of various biomolecules, including enzymes, antibodies and biosensors. This knowledge will enable them to seek advanced courses and professions related to pharmacology and bioanalytical chemistry.

## **Evaluation Pattern – R.13 & R.16**

**Course Outcomes**

The course enables the students to

**CO 1:** Understand the role of aminoacids, proteins and peptides in biology along with their application.

**CO 2:** Describe the basic properties, mechanisms of action and applications of enzymes

**CO 3:** Gain knowledge in nucleic acids, antibodies, recombinant DNA and gene analyses.

**Course Contents:****Unit 1 Amino acids, Proteins and Peptides**

Classification, Stereochemical aspects, physical properties, Ionic properties, spectral properties, essential and non essential amino acids, chemical reactions of amino acids, Industrial preparation and chemical synthesis of amino acids. Ionic properties of proteins, protein structure, protein purification, protein structure determination, proteomics and protein function, solid phase peptide synthesis, biologically important peptides.

**Unit 2 Enzymes**

Introduction to Enzymes, Classification of enzymes, mechanism of enzyme action, immobilized enzymes and enzyme technology, enzyme analog built polymers, design of molecular clefts, enzymes in synthetic organic chemistry. Enzymes in biological systems

**Unit 3 Molecular biology and bioinformatics**

Structure of nucleic acids, genes and genome complexity, functions of nucleic acids, isolation and separation of nucleic acids, molecular analysis of nucleic acid sequences, nucleotide sequencing of DNA.

**Unit 4 Immunochemical techniques**

Production of antibodies, purification and fragmentation of immunoglobulins, immunoprecipitation, labeling antibodies, immunoblotting, immunoassays, immunohisto/cytochemistry.

**Unit 5 Recombinant DNA and genetic analysis**

Constructing gene libraries, cloning vectors, hybridization and gene probes, application of gene cloning, expression of foreign genes, pharmacogenomics.

**REFERENCES:**

1. Hermann Dugas, 'Bioorganic Chemistry - A Chemical Approach to Enzyme Action', 3<sup>rd</sup> edition, Springer.
2. Keith Wilson and John Walker, 'Principles and Techniques of Biochemistry and Molecular Biology', 6<sup>th</sup> edition, Cambridge University Press.

**Learning Outcomes:** This course provides the students with detailed information about the chemistry enzymes, proteins and peptides. It also familiarises students with immunochemical techniques, genetic analysis and bioinformatics. This knowledge will enable them to seek advanced courses and professions related fields.

**Evaluation Pattern – R.13 & R.16****Course Outcomes**

The enables the students

**CO 1:** To gain knowledge about various water treatment processes adopted in industries

**CO 2:** To get an in-depth overview on production, refining and processing of various types of fuels

**CO 3:** To understand the importance and preparative methods of explosives and chemical weapons

**CO 4:** To learn the manufacturing process of paints and pigments and to develop ability to scale up the products prepared in the laboratory to the industrial level

**CO 5:** To obtain a comprehensive knowledge of various energy resources used commercially

**CO 6:** To calculate, analyse and execute different types of industrial processes

### **Course Contents:**

#### **Unit 1 Water treatment**

Softening of water, Ion exchange process, Lime soda process, Modified Lime soda process, Zeolite process, Chemical and physical method of sterilization, Desalination, Boiler problems. Corrosion of boiler units, industrial water treatment, water analysis.

#### **Unit 2 Fuels**

Calorific value, determination of Calorific value, classification of fuels, Solid fuels, Properties of fuels, classification of coal, coking and non-coking coals, advantages and disadvantages of solid fuels. Liquid fuels, gaseous fuels, analysis of fuel gases, Distillation of petroleum. Processing & purification of petroleum and petroleum products, Flash point, Fire point, Knocking, antiknocking, Cetane number, octane number, natural gasoline, cracking, polymerization, alkylation, isomerisation, rocket fuels, fossil fuels, nuclear fuels.

#### **Unit 3 Energy resources**

Renewable and non-renewable sources of energy, conventional and non conventional sources of energy, solar energy, solar technology, solar photovoltaic cell - application, PV lantern system, Radiotelephone system, Application of solar energy, Environmental implication, Nuclear energy, nuclear fuel cycle in India, Energy conservation and waste heat boilers, Fuel cells, hydrogen cells.

#### **Unit 4 Paints and Pigments**

White pigment, blue, green, yellow, black and red pigments - manufacture, physical properties, characteristics, Manufacture of paints, setting of paints, requirement for good paints, emulsion paint, latex paint, luminescent paint, fire retardant paints, heat resistant paints, varnishes, manufacture of varnishes, enamels, lacquers.

#### **Unit 5 Explosives and Toxic Chemical Weapons**

Introduction, Classification. Deflagrating or low explosives. Characteristics of explosives, nitrocellulose, PETN, DNB, TNB, TNT, Picric Acid, Nitrogllycerine, Dynamite, Cirdite, Gun powder, RDX, EDNA, HMX, Tetryl, Pentryl, Hexyl, Dinol. Toxic chemical weapons, screening smokes, Incendiaries, Pyrotechniques, Explosives in India.

### **TEXTBOOKS:**

1. B. K. Sharma, 'Industrial Chemistry', Goel publishing.
2. James A Kent, 'Riegels Hand book of Industrial chemistry', 10<sup>th</sup> edition, Kluwer Academic/Plenum publishers, 2003.

### **REFERENCES**

1. Alan Heaton, 'An Introduction to Industrial chemistry', 3<sup>rd</sup> edition, Blackie Academic and professional, 1996.
2. Chris A Clausen and Guy Mattson, 'Principles of industrial chemistry', 2<sup>nd</sup> edition Wiley, 1978.
3. Jonathan Steed, 'Core Concepts on supramolecular chemistry and nanochemistry', Wiley Eastern Publishers, 2006.

**Learning Outcomes:** This course familiarises the students with the various industrial processes and products, including energy storage materials, paints, explosives. The detailed understanding of these things is necessary to secure a career in the chemical industries.

## Evaluation Pattern – R.13 & R.16

**18CHY635                      INDUSTRIAL STOICHIOMETRY                      3 0 0 3**

### Course Contents:

**Unit 1** Introduction to process calculation - dimensions and systems of units - fundamental quantities of units, derived quantities, definition and units of force, volume, pressure, work, energy, power, heat-unit conversions in FPS, MKS and SI systems.

**Unit 2** Mixtures and solutions - methods of expressing compositions of mixture and solutions, wet and dry basis concept. Ideal and real gas laws – Gas constant – normal molal volume, calculations of pressure, volume and temperature using ideal gas law. Gas mixtures – Use of partial pressure and pure component volume in gas calculations. Dissociating gases. Relation between mole%, volume% and pressure% of ideal gases calculation of average molecular weight, density, mole%, weight% in gas mixture in SI/MKS systems – applications of real gas relationship in gas calculation.

**Unit 3** Description and simple material balance calculation of physical processes such as drying, distillation, absorption, mixing, crystallization, Evaporation.

**Unit 4** Single stage material balance calculation of leaching and extraction, calculations involving recycling and bypassing operation - limiting reactant, excess reactant, conversion, yield and selectivity - simple numerical for finding yield, conversion and composition.

**Unit 5** Calculation of material and energy balance based on reactions involving heat capacity and specific heat - mean heat capacity of gases - heat capacity of gas mixture and liquid mixture. Calculations of heat capacity by integral equation up to three terms - sensible and latent heats of fusion, sublimation, vaporization. Calculations of standard heat of formation from heat of combustion data. Calculations for heat of reaction from heat of formation and heat of combustion data – Fuels - calorific values proximate and ultimate analysis - air requirement and composition of flue gases.

### TEXTBOOKS:

1. Bhatt, B. L. Vora, S. M., “Stoichiometry”, 3<sup>rd</sup> Edition, Tata McGraw-Hill (1996).
2. Felder, R. M. and Rousseau, R. R. “Elementary Principles of Chemical Processes” 3<sup>rd</sup> Edn., John Wiley & Sons, New York 2000.

### REFERENCE BOOKS:

1. Hougen O.A., Watson K.M. and Ragatz R.A., “Chemical Process Principles” Part I, CBS Publishers (1973).
2. Warren, K Lewis, Arthur H. Radash & H. Clay Lewis, “Industrial Stiochiometry”, McGraw Hill Book C., NY 1995.

**Learning Outcomes:** This course re-introduces the concepts of stoichiometry with respect to the important industrial processes. The knowledge and understanding of industrial stoichiometry are necessary to secure a career in the chemical industries.

## Evaluation Pattern – R.13 & R.16

**18CHY636                      MATERIAL SCIENCE AND NANOCHEMISTRY                      3 0 0 3**

## Course Outcomes

After completing the course, students gain a

**CO 1:** Perfect understanding of nanomaterials, their preparation and properties.

**CO 2:** Basic knowledge in classification and quantum confinement

**CO 3:** A sound understanding of characterization techniques

**CO 4:** Wide knowledge in the application of nanomaterials in different arenas.

**CO 5:** a thorough knowledge of the fate of nanomaterials in the environment as well as living organisms and the ethical use of nanomaterials

## Course Contents:

**Unit 1** Introduction to Nanomaterials Introduction to Material Science, Interdisciplinary nature, Structure of nanomaterials, Length scales, de-Broglie wavelength & exciton Bohr radius, Foundations of Quantum Mechanics: wave function, Schrödinger equation, uncertainty principle, quantum wells, quantum wires, quantum dots, articles.

**Unit 2** Nanomaterials: Synthesis, Properties Size effect and properties of Nanoparticles - Particle size - Particle shape - Particle density, Specific surface area and pore - Composite structure, Crystal structure - Functionality of nanostructures and their characteristic evaluation - Optical properties - Catalytic property; Synthesis - Methods and Strategies, Top-down and bottom-up approaches, Chemical vapor deposition, Laser ablation, Electric-arc, Sol-Gel Processing, Lithography - Surface modification of inorganic nanoparticles by organic functional groups.

**Unit 3** Surface Science and Characterization of Nanomaterials Electron Microscopy, MFM, SNOM, SEM, TEM, EDAX, X-ray Diffraction and Electron diffraction, Atomic Force Microscopy, Scanning Tunneling Microscopy, Spectroscopy: UV-Visible spectroscopy, Photoluminescence spectroscopy, IR spectroscopy, FTIR and ATR, Raman spectroscopy, Self-Assembled Monolayers.

**Unit 4** Nanotechnology: Applications and Devices Nanoscale materials, Nano transfer printing, Biomaterials applications, MEMS and NEMS, selforganisation, nanoscale (opto) electronics, Fullerenes, Devices - Actuators and motors for nanodisplacements, Nanosensors, development of optical memory using semiconductor nanoparticles - Nozzle-free inkjet technology - Dendrimers and their application to organic electronics devices - Nanomedicines, Bio-imaging with quantum dots.

**Unit 5** Environmental Issues in Nanotechnology Nanoparticles and environment - Nanoparticles in atmosphere - Ground water, exhaust gases – wastewater and Indoor environments; Safety of nanoparticles - Problems caused by nanoparticles, Safety assessment for the nanoparticles; Removal of nanoparticles.

## TEXTBOOKS:

1. T. Pradeep, 'Nano - The Essentials Understanding Nanoscience and Technology', McGraw-Hill Professional Publishing, 2008.
2. Charles P. Pool and Frank J. Ovens, 'Introduction to Nanotechnology', John Wiley and sons, 2006.

## REFERENCES:

1. Ozin, Geoffrey Alan, Arsenault, 'Nanochemistry: A Chemical Approach to Nanomaterials', Royal Society of Chemistry, 2008.
2. C.N.R. Rao, A.Muller, A.K.Cheetham, 'The Chemistry of Nanomaterials: Synthesis, Properties and Applications', Wiley-Vch Verlag Gmbh & Co., 2004.
3. Alexei Nabok, 'Organic and Inorganic Nanostructures', Artech House, 2005.
4. C. Richard Brundle, Charles A. Evans Jr., and Shaun Wilson, 'Encyclopedia of Materials Characterization', Butterworth-Heinemann Publishers, 1992.



5. Masuo Hosokawa, Kiyoshi Nogi, Makio Naito and Toyokazu Yokoyama, 'Nanoparticle Technology Handbook', Elsevier Publishers, 2007.

**Learning Outcomes:** This course provides the students with complete knowledge of nanomaterials, synthesis, structures, their characterizations and specific applications. This knowledge is essential for the students to continue their studies or research in the nanochemistry and nanotechnology, it will also be very useful in seeking a profession in related sector.

## Evaluation Pattern – R.13 & R.16

18CHY637

MEDICINAL CHEMISTRY

3 0 0 3

### Course Outcomes

The course helps the students

**CO 1:** To understand the physicochemical properties of drug and its metabolic pathways, adverse effect and therapeutic value of drugs.

**CO 2:** To know the role of enzymes and vitamins in biological action.

**CO 3:** To understand the chemistry of various drugs with respect to their pharmacological activity

### Course Contents:

**Unit 1 Medicinal chemistry:** Introduction, drugs – classification of drugs – mechanism of drug action. Drug-receptor complex, nomenclature – agonist.

**Unit 2 Physicochemical properties of drugs in relation to biological action:** solubility, Partition coefficient, dissociation constant, hydrogen bonding, ionization, drug shape, surface activity, complexation, protein binding, molar refractivity, bioisosterism – stereo chemical aspects of drug action.

Enzymes, hormones and Vitamins - representative cases, nomenclature, classification and characteristics of enzymes, mechanism of enzyme action, factors affecting enzyme action, co-factors and co-enzymes, enzymes in organic synthesis, mechanism of enzyme catalysis, enzyme inhibition. Hormones and vitamins – representative cases.

### Unit 3 Essentials of drug design

Molecular mimetics, drug-lead modification, drug design using QSAR and computer assisted design, assessment of drug activity, receptors and drug action, mechanism of drug action, drug metabolism pathways, Drug potentiation, drug antagonism and drug resistance

### Unit 4 Medicinal agents from natural products

History of the use of natural products as therapeutic agents, medicinal plants, active principle, Isolation methods of alkaloids, terpenes, antioxidants, natural oils from plants.

### Unit 5 Medicinal agents

Medicinal agents belonging to alkaloids, steroids, polypeptides, modified nucleic acid bases, sulphonamide and sulpha drugs, antibacterials - sulpha drugs, substituted sulphonamides, anticonvulsants, anticoagulants, antiamoebic agents, antihelmintic agents, anti-malarial agents, diuretics and cardio vascular agents, medicinal agents affecting CNS, analgesics, antipyretics, antiseptics and disinfectants, Histamine and anti-histaminic agents.

Infectious and non-infectious diseases (malaria, AIDS, Cancer) introduction, mechanism of action types of cure.

### TEXTBOOKS:

1. John M beak and John H Block, 'T Wilson, O. Gisvold and R. F. Deorge - Text book of Organic,

*Medicinal and Pharmaceutical Chemistry*, 7<sup>th</sup> edition, J.B. Lippincott Williams and Wilkins Company, 1977.

2. A.Burger, *'Medicinal Chemistry'*, 3<sup>rd</sup> edition, Wiley Interscience, 1970.
3. V.K.Ahluwalia and Madhu Chopra, *'Medicinal Chemistry'*, Ane Books pvt Ltd, 2008.

#### **REFERENCES**

1. V.Koethekar, *'Essentials of Drug Designing'*, 14<sup>th</sup> edition, Dhruv publications, 2005.
2. V.K.Ahluwalia, Lalita S.Kumar and Sanjiv Kumar, *'Chemistry of Natural Products'*, Ane Books India.
3. L.P.Graham *'An introduction to Medicinal Chemistry'*, 3<sup>rd</sup> edition, Oxford University Press, 2005.

**Learning Outcomes:** This course provides the detailed information about the medicinal drugs, physicochemical properties of drugs in relation to biological action, drug design, and extraction of medicinal agents from natural products. This knowledge is essential for the candidates who wants to continue in medicinal chemistry or pharmacology for higher studies, reaserch or a career.

#### **Evaluation Pattern – R.13 & R.16**

**18CHY638**

**SUPRAMOLECULAR CHEMISTRY**

**3 0 0 3**

#### **Course Outcomes**

The course enables the students

**CO 1:** To understand the basic concepts of molecular and supramolecular chemistry. Understand the bottom-up and top-down approach used for the synthesis of supramolecular assemblies.

**CO 2:** To learn about fundamental principles of photoinduced charge transfer and energy transfer, molecular electronics, molecular photonics etc.

**CO 3:** To understand the underlying principles of molecular recognition, semiochemistry , get to know various receptors like crown ethers, cyclophanes, cyclodextrins etc

**CO 4:** To familiarise with electrochemically controllable molecular switchable systems

**CO 5:** To familiarise with molecular scale mechanical devices, molecular motors, allosteric movements, tweezers, harpoons, molecular rotaxanes, catenanes and threading and dethreading movements associated with them

#### **Course Contents:**

##### **Unit 1 Introduction to Supramolecular Chemistry**

From molecular to supramolecular chemistry: Factors leading to strong binding, hydrogen bonding and stacking interactions, Bottom-up approach, Top-Down Approach, Energy and Signals Semiochemistry, photo switching devices, electro switching devices, mechanical switching processes.

##### **Unit 2 Processing of Energy and Signals by Molecular and Supramolecular system**

Fundamental principles of photo induced electron and energy transfer, Molecular electronics, Molecular photonics, Molecular Chemionics, Molecular electro photonics, Molecular Photochemionics.

##### **Unit 3 Molecular Recognition**

Molecular receptors: crown ethers, siderophores, cyclophanes, cyclodextrin and their application in specific recognition processes. Metal guided self assembly reactions, molecular knot with double helical complexes, Self assembly of polynuclear metal complexes.

##### **Unit 4 Electrochemistry of Supramolecular Systems**

Electroluminescent systems as sensors and devices, Redox controlled molecular switches, Biohybrid electrochemical devices, Dendrimers as multielectron storage devices, Redox-active Metal-Polypyridinedendrimers as light harvesting antennae.

**Unit 5 Molecular Scale Mechanical Devices** Introduction to mechanical devices, Spontaneous mechanical like motions, Allosteric movements, Tweezers and Harpoons, A natural proton pump, Twisters, Tweezers, Threading-Dethreading movements, Ring switching processes in Rotaxanes and Catenanes, Molecular valves, Molecular Muscles.

**TEXTBOOKS:**

1. Vincenzo Balzani, 'Supramolecular Chemistry', Kluwer Academic, 1992
2. Vincenzo Balzani, Alberto Credi and Margherita Venturi, 'Molecular Devices and Machines: A Journey Into the Nanoworld', Wiley, 2006.
3. Paola Ceroni, Alberto Credi and Margherita Venturi, 'Electrochemistry of Functional Supramolecular Systems', Wiley, 2010.

**REFERENCES:**

1. Jonathan W. Steed Atwood, Jerry L. Chich, 'Supramolecular Chemistry', 2<sup>nd</sup> edition, Wiley, 2009.
2. Fritz Vögtle and F. Alfter 'Supramolecular Chemistry: An Introduction', John Wiley & Sons, 1999.
3. Jean-Marie Lehn, 'Supramolecular Chemistry', RCS pubs., 2005
4. Jonathan Steed, David Turner and Carl Wallace, 'Core concepts in Supramolecular Chemistry and nanochemistry', John Wiley & Sons, 2007
5. Katsuhiko Ariga and Toyoki Kunitake, 'Supramolecular chemistry – Fundamentals and applications advanced textbook', Springer-Verlag, 2000.

**Learning Outcomes:** This course provides detailed information about the theories and concepts of supramolecular chemistry. Students get to learn about the processing of energy and signals by molecular and supramolecular systems, molecular recognition, electrochemistry of supramolecular systems, and molecular scale mechanical devices. This knowledge is useful for the students to understand and advance in the area of supramolecular chemistry.

**Evaluation Pattern – R.13 & R.16**

18CHY639

Nanomaterials for Biomedical Applications

3 0 0 3

**Course Contents:**

**Unit 1:** Introduction to Nanomaterials: Size dependence of properties – Surface to volume ratio and Quantum confinement. Microscopic techniques to study nano structures - SEM, AFM – TEM and STM. Spectroscopic techniques to characterize nanostructures - Raman, XPS, Auger, EDAX.

**Unit 2:** Synthetic approaches: Colloidal, Self-Assembly (Self assembled monolayers-SAMs) and electrostatic self-assembly, electrochemical methods (cathodic and anodic processes), sol-gel, Langmuir-Blodgett (LB) technique, chemical vapour deposition, plasma arcing and ball milling, lithography.

**Unit 3:** Electrical, optical, mechanical, chemical and magnetic properties of nanomaterials. Surface Plasmon resonance – Fluorescence Resonance energy transfer (FRET).

**Unit 4:** Carbon Clusters: Synthesis, properties and biomedical applications of Fullerenes, Carbon nanotubes and Graphenes. Quantum Dots, wells and wires (metallic and semiconducting) - Preparation, properties and biomedical applications. Dendrimeric structures and their applications.

**Unit 5:** Biofunctionalisation of nanomaterials - Noncovalent Assembly - Covalent assembly - Biofunctional Nanomaterials - Semiconductor Nanoparticles - Magnetic Nanoparticles. Applications of Biofunctional nanomaterials – Optical and Electrochemical Sensing.

#### REFERENCES:

1. Alexei Nabok, “Organic and Inorganic Nanostructures”, Artech House, Inc., 2005
2. Huangxian Ju, Xueji Zhang and Joseph Wang, “NanoBiosensing, Principles, Development and Application”, Springer, 2011.
3. M. Reza Mozafari (Editor), “Nanomaterials and Nanosystems for Biomedical Applications”, Springer 2007.
4. Zhong Lin Wang (Editor), “Characterisation of Nanophase Materials”, Wiley VCH, 2000.

**Learning Outcomes:** This course provides the detailed information about the nanomaterials that have versatile biomedical applications. The students learn about the synthesis, properties, characterization and biofunctionalization of nanomaterials. This knowledge is essential for the students to go for the advanced courses or career related to nanotechnology and non-medicine.

### Evaluation Pattern – R.13 & R.16

**18CHY640**

**INDUSTRIAL METAL FINISHING PROCESSES**

**3 0 0 3**

#### Course Contents:

**Unit 1** Background Theory: Review of reversible and irreversible processes - electrodes, indicator and reference - Nernst and Butler-Volmer equation - phenomenon of polarization - factors influencing - Tafel experiment and Tafel plot - Significance.

**Unit 2** Electrodeposition: Industrial plating of copper-nickel (dull and bright) - chromium on mild steel – operating conditions and sequence – pre-treatment processes - plant layout – electroplating of zinc on MS and post plating chromating, yellow and blue passivation processes – decorative plating of silver and gold on non-ferrous metals – brief discussion on nano plating of metals and micro structure of the deposition. Properties of deposits: Tests for adhesion, hardness, thickness, uniformity and corrosion resistance of the electro deposits.

Electroless deposition: Nickel, copper, gold on metal components – bath composition and operating conditions - immersion plating - plating on plastics – pre-treatment processes – long duration plating – electroforming, operating conditions and sequence.

**Unit 3** Anodising: Industrial anodizing of aluminium and its alloys – baths used, operating conditions and sequence – plant layout – effect of temperature and current density on the thickness of anodic film – determination of thickness – industrial applications.

Nano anodizing of titanium, aluminium and tantalum – application to sensor field.

Plasma electrolytic oxidation: power supply requirements – baths used – process sequence for aluminium, magnesium and titanium – properties of the coating and industrial applications.

**Unit 4** Electropolishing: Mechanism of electropolishing – electropolishing of ferrous and non-ferrous metals – industrial baths used – operating conditions and sequence - industrial applications.

**Unit 5** Electrochemical etching: Etching of ferrous and non-ferrous metals – special properties of matt and satin finish – DC and AC processes – operating conditions and sequence.

Special Topics: Electrochemical and chemical metal colouring of ferrous and non-ferrous metals.

Black nickel coating – Hard chromium deposition – Hard anodizing of aluminium – Electrochemical

machining of hard steels – Electro-winning process – Barrel plating – Electrodeposition of paint.

**TEXTBOOK:**

1. Derek Pletcher and Frank C. Walsh, 'Industrial Electrochemistry', Blackie Academic and Professional, (1993).

**REFERENCES:**

1. Christopher M A, Brett, 'Electrochemistry – Principles, Methods and Applications', Oxford University, (2004).
2. Watanabe T, 'Nano-plating: microstructure control theory of plated film and data base of plated film microstructure', Elsevier, Oxford, UK (2004).
3. Kanani N, 'Electroplating and electroless plating of copper and its alloy', ASM International, Metals Park, OH and Metal Finishing Publications, Stevenage, UK (2003).
4. Curtis, 'Electroforming', London, (2004).
5. Rumyantsev E and Davydov A, 'Electrochemical machining of metals', Mir, Moscow, (1989).
6. Peter G Sheasby 'Basics of aluminium anodising', Banbury, Oxon (2001)
7. Robert Brugger 'Nickel Plating' Robert Draper Ltd, Teddington, (1970)
8. J.K.Dennis, T.E.Such, 'Nickel and Chromium Plating, Third Edition' Woodhead Publishing Series in Metals and Surface Engineering, 3rd Edition, (1993)

**Learning Outcomes:** The wide and indepth knowledge the students get in this course about the industrial metal finishing processes is very useful for them to secure a job in the related industries.

**Evaluation Pattern – R.13 & R.16**

**18CHY641**

**Biosensors: Fundamentals and Applications**

**3 0 0 3**

**Course Contents:**

**Unit 1:** Introduction to biosensor – classification based on the signal transduction and biorecognition element. Enzymatic and non-enzymatic sensors, DNA and protein based sensors-immunosensors.

**Unit 2:** Biosensing using nanomaterials: Concepts of surface to volume ratio, quantum confinement, surface plasmon resonance, fluorescence, chemiluminescence and electroluminescence and FRET in biosensing. Application of metal, semiconducting quantum dots, carbon nanotubes, graphene and carbon dots in biosensing.

**Unit 3:** Electrochemical principle in biosensing: Principles of potentiometry, voltammetry, amperometry and impedimentary in biosensing. Principle, fabrication and working of optical, electrochemical biosensors. Construction and working of potentiometric, amperometric and impedemetric sensors. Development and applications of piezoelectric sensors.

**Unit 4:** Optical and electrochemical sensors for glucose, vitamins, cholesterol, dopamine, nitric oxide, nitrates, and pesticides. Biocompatibility of sensors.

**Unit 5:** Biochips and wearable devices: lab-on-a-chip - fabrication of microfluidics- lithography, wearable sensors, epidermal electronic system, lab-on-skin-devices.

**REFERENCES**

1. Xueji Zhang, Huangxian Ju, Joseph Wang, "Electrochemical Sensors, Biosensors and Their Biomedical Applications", Elsevier, 2008
2. Joseph Wang, "Analytical Electrochemistry", Wiley, 2006

3. Huangxian Ju, Xueji Zhang, Joseph Wang, "NanoBiosensing: Principles, Development and Application", Springer, 2011.
4. Peter Grundler, "Chemical Sensors – An Introduction for Scientists and Engineers", Springer-Verlag, Berlin Heidelberg, 2007
5. Arben Merkoci, "Biosensing using nanomaterials" Wiley, 2009.

**Learning Outcomes:** This course deals with the fundamentals and applications of biosensors, students get to learn about the electrochemical and optical biosensors, biochips and wearable devices. This knowledge will help the students to advance further into the biosensor field either for R&D or production career.

## Evaluation Pattern – R.13 & R.16

18CHY642

Computational Chemistry

3 0 0 3

### Course Outcomes

This course helps students to gain

**CO 1:** Knowledge on approximation methods

**CO 2:** Ability to apply approximation methods

**CO 3:** Knowledge on potential energy surface

**CO 4:** Ability to apply potential energy surface

**CO 5:** Theoretical knowledge on the various tools or methods of Computational Chemistry

**CO 6:** Knowledge of application of various tools or methods of Computational Chemistry

**CO 7:** Knowledge on basis sets

**CO 8:** Knowledge on orbitals

### Course Contents:

#### Unit 1 - Introduction

Introduction to computational chemistry (molecular modelling), questions commonly investigated computationally, principle and application of methods (tools) of computational chemistry - molecular mechanics, ab initio method, semiempirical methods, density functional theory and molecular dynamics, STOs, GTOs, basis sets, specification of molecular geometry using Cartesian coordinates and internal coordinates, Z-matrix, Z-matrix of simple molecules (water, ethanol), potential energy surface (PES), potential energy surface of diatomic molecules and triatomic molecules (H<sub>2</sub>O and HOF) - hypersurface and process of "slicing", stationary points on a potential energy surface - potential energy surface of the isomerization reaction of ozone to isoozone, stationary points (ozone, isoozone and transition state), intrinsic reaction coordinate, minimum, relative minimum, saddle-shaped surface, saddle point, higher-order saddle point and mathematical treatment of stationary points, Born-Oppenheimer approximation and its significance and frozen-nuclei energy.

#### Unit 2 - Molecular Mechanics

Introduction to molecular mechanics, forcefield, developing a force field - expression for potential energy of a molecule, bond stretching term, angle bending term, torsional term and nonbonded interaction term, parameterizing a forcefield - parameterizing bond stretching term, angle bending term, torsional term and nonbonded interaction term, calculation using forcefield - compare the energies of two 2, 2, 3, 3-tetramethylbutane geometries, illustration of application (use) of molecular mechanics - calculation of

geometries and energies of small-sized and medium-sized molecules, polymers and transition states (transition state for the Diels-Alder reaction of butadiene with ethene to form cyclohexene), in organic synthesis for predicting the more suitable path for carrying out the synthesis and calculation of normal-mode vibrational frequencies for characterizing a species as a minimum or a transition state or higher-order saddle point, for obtaining zero-point energies to correct frozen-nuclei energies and for interpreting or predicting IR spectra, strength (merit) and weakness (demerit) of molecular mechanics.

### Unit 3 - Semiempirical methods - Part 1

Introduction to semiempirical (SE) methods, Simple Huckel Method (SHM) - theory - expression for calculating energy of a molecular species, expression for molecular wave function based on LCAO approximation, secular equations and the single matrix equation, H, C, S and  $\epsilon$  matrices and their interpretation, the values of  $H_{ij}$  as zero, coulomb integral  $\alpha$  and bond integral  $\beta$  and their physical significance, the H matrix in terms of  $\alpha$ ,  $\beta$  and zero for ethene system (ethene neutral molecule, ethene radical cation and ethene radical anion), propenyl system (propenyl cation, propenyl neutral radical and propenyl anion) and cyclobutadiene system (square cyclobutadiene dication, square cyclobutadiene neutral molecule and square cyclobutadiene dianion), the H matrix in terms of zero,  $\alpha = 0$  and  $\beta = -1$  for ethene systems (ethene neutral molecule, ethene radical cation and ethene radical anion), propenyl system (propenyl cation, propenyl neutral radical and propenyl anion) and cyclobutadiene system (square cyclobutadiene dication, square cyclobutadiene neutral molecule and square cyclobutadiene dianion), result of diagonalization of the H matrices written for ethene system, propenyl system and cyclobutadiene system, molecular orbital energy level diagrams and expressions for energy and molecular wave functions for ethene system, propenyl system and cyclobutadiene system based on the result of diagonalization of the H matrices, and molecular orbital energy level diagrams for ethene system, propenyl system and cyclobutadiene system showing ground state and excited state electronic configurations.

### Unit 4 - Semiempirical methods - Part 2

Application of SHM - nodal properties of molecular orbitals and Woodward-Hoffmann orbital symmetry rule, stability towards oxidation and reduction of various species in ethene system, propenyl system and cyclobutadiene system, geometry of cyclobutadiene molecule as predicted by SHM and its Jahn-Teller distortion, aromaticity and Huckel's  $(4n + 2)$   $\pi$  electron rule, and calculation of resonance (stabilizing) energy, bond order and atomic charges of various species in ethene system, propenyl system and cyclobutadiene system, strength of SHM, weakness of SHM (detailed explanation) - basis set is limited to p orbitals ( $p_z$  orbitals), it treats only  $\pi$  electrons, and the overlap integrals, Fock matrix elements, electron spin and electron-electron repulsion are not calculated/accounted properly, Extended Huckel Method (EHM) - minimal valence basis set, calculation of Fock matrix elements, and calculation of overlap integrals by Lowdin orthogonalization, EHM procedure, EHM calculation on protonated helium molecule, application of EHM - an overall idea, strength and weakness of EHM, SCF SE methods - Pariser-Parr-Pople (PPP) method and Complete Neglect of Differential Overlap (CNDO) method - basic principle (an exhaustive treatment is **not** expected).

### Unit 5 - Density Functional theory and ab initio method

(An exhaustive treatment is **not** expected)

Introduction to Density Functional theory and calculations, Kohn-Sham approach - the first and the second Hohenberg-Kohn theorems, introduction to ab initio method and calculation, basis sets for H, He and first, second and third row elements used in ab initio calculations - STO-3G, 3-21G, 3-21G(\*) and 6-31G\*, these basis sets for a few molecular species (water, methane and carbene), basic principles of ab initio method (an idea only).

### Text Book

1. Computational Chemistry-Introduction to the Theory and Applications of Molecular and Quantum Mechanics - Errol Lewars

**Learning Outcomes:** This course introduces the students with the concepts of computational chemistry. Students will learn about the molecular mechanics, semi-empirical methods, Density functional theory and ab initio method. This theory knowledge is essential for to students to advance in the chemistry related

fields either for research or a job.

## Evaluation Pattern – R.13 & R.16

18CHY643

Sustainable Chemical Science

3 0 0 3

### Course Contents:

#### Unit 1 Green Chemistry and Sustainability

History of green chemistry, Chemical composition of the, environment (Air, water & soil- Role of organic and inorganic molecules in pollution), the twelve principles of green chemistry (detailed description with examples), green chemistry as an expression of environmental ethics (Thrift Chemistry), the concept of sustainability, from green to sustainable chemistry, sustainable use of chemical feedstock, water and energy, quantifying greenness of a chemical reaction, green chemistry metrics- mass based, energy and environmental metrics, designing greener process, life cycle assessment (introduction and scope), Green toxicology- the need, principles of toxicology, Disposition of Toxicants in Organisms, Non-Organ System Toxicity, Mechanistic Toxicology, Quantitative Structure–Activity Relationships, (Environmental Toxicology-Persistence and bioaccumulation), Non-Cancer risk assessment, Cancer risk assessment, stakeholders in sustainable policy implementation.

#### Unit 2 Chemistry in water

Definition and attributes of a green solvent, the principle and reasons for use of water in green chemistry- hydrophobicity- cyclodextrin chemistry, Lewis acids in aqueous media, Michael addition in water using triflates, green processes with base in water, green oxidations and reduction in water, on water conditions, use of water in microwave and ultrasonic technology.

#### Unit 3 Green solvents

Ionic liquids as green solvents- definition and notation- properties, synthesis and use in organic reactions, oxidation, oxidative carbonylation of aniline, Friedel–crafts reaction, Michael addition, Fischer Indole synthesis, Benzoin condensation, dimethyl carbonates synthesis in ionic liquids. Super critical fluids- super critical water and carbondioxide- properties and organic transformations.(Diels Alder, Clasen rearrangement, Fisher Indole, Friedel–crafts reaction, oxidation and hydrogenation. Properties and application in organic transformation of green solvents like polyethylene glycol, glycerol, cyclopentyl methyl ether, 2-methyltetrahydro furan, Perfluorinated (Fluorous) Solvents- Fluorous Biphase Concept and dimethyl carbonate.

#### Unit 4 Green Chemistry and Catalysis

Importance of catalysis, turn over number and frequency, the basis of catalysis-kinetic phenomenon, basics of homogeneous, heterogeneous and biocatalysis, sabatier's principle, catalyst -deactivation, sintering, thermal degradation, inhibition and poisoning, catalyst promoters, modifiers, supported catalysts and reagents for green chemistry- heterogenized reactions for green chemistry, preparation of solid catalyst-slurry and co-precipitation, impregnation, hydrothermal synthesis- drying, calcination, activation and forming, selecting the right support, catalyst characterization- surface characterization methods, temperature programmed techniques, spectroscopy and microscopy. Common mechanism in enzyme catalysis immobilized enzymes, developing biocatalyst- rational design and directed evolution, non-enzymatic biocatalysts.

#### Unit 5 Green Chemistry Technologies and Alternate Energy Sources

Design for Energy Efficiency, Photochemical Reactions Advantages of and Challenges Faced by Photochemical Processes (Examples). Microwaves as energy source in chemistry- properties of microwaves, microwave heating (Effects), Approaches to Microwave-assisted Organic Chemistry- solvent free methods, MORE chemistry, continuous microwave reactor (CMR)-microwave batch reactor (MBR), examples of organic transformations. Sonochemistry and Green Chemistry-Theoretical Basis- Cavitation Inception,



Nucleation-Bubble Dynamics- examples of organic transformations, Sono-chemical synthesis of nano-structured materials, Electrochemical Synthesis- materials manufactured using the process, organic electrosynthesis- 3-bromothiophen from thiophene. Renewable Sources of Energy, Solar Energy, Wind Power, Geothermal Solution, Hydropower (Sources, Merits and Difficulties in widespread applications), Indian Energy scenario- Energy Conservation act (2001)- features.

## Reference

1. Green chemistry and engineering A Pathway to Sustainability, Anne E. Marteel-Parrish, Martin A. Abraham, American Institute of Chemical Engineers, Inc, John Wiley & Sons, Inc 2014.
2. Synthetic organic Sonochemistry, Jean-Louis Iuche, Springer Science+Business Media New York, 1998
3. New Methodologies and Techniques for a Sustainable Organic Chemistry, Alessandro Mordini and Ferenc Faigl, Springer, 2008.
4. Green chemistry, Fundamentals and Applications, Suresh C. Ameta and Rakshit Ameta, CRC press, Taylor & Francis Group, 2013
5. Handbook of Green Chemistry, Vol5 Green Solvents- Reactions in Water, Paul T Anastas, Chao Jun Li
6. Sonochemistry: theory, reactions, syntheses, and applications, Filip M. Nowak, Nova Science Publishers, Inc, 2010.
7. Green Chemistry Metrics, A Guide to Determining and Evaluating Process Greenness, Dicks, Andrew, Hent, Andrei, SpringerBriefs in Green Chemistry for Sustainability, 2015
8. Catalysis: concepts and applications, Gadi Rothenberg, Wiley-VCH Verlag & Co. KGaA, Weinheim, Germany, 2008

**Learning Outcomes:** In this course, the students learn about green chemistry and sustainability, green solvents, green chemistry and catalysis, green chemistry technologies and alternate energy sources. The knowledge and they get in this course will be useful for them to continue their studies in the related fields or to land a profession.

## Evaluation Pattern – R.13 & R.16

18CHY644                      Sustainable Techniques in Chemical Sciences                      3 0 0 3

### Course Contents:

#### Unit 1 From Industrial to Sustainable Chemistry

Industrial Sustainable Chemistry- Managing Intraorganizational Sustainability, Managing Horizontal Interorganizational Sustainability, Managing Vertical Interorganizational Sustainability. Integrated Pollution Prevention and Control- Best Available Techniques reference documents (BREFs), From Industrial Emissions Directive (IED) to Voluntary Systems, Policy Drivers for Sustainable Chemistry (Transition Concept), Development of a CSR Management System Framework. Sustainability Assessment Methods and Tools- Sustainability Assessment Framework, Impact Indicators and Assessment Methodologies, Environmental Impact Assessment, Economic Impact Assessment, Social Impact Indicators, Understanding Industrial Symbiosis-Cluster Management. Sustainability of Logistics in the Chemical Sector, Basic Principles of Chemical Leasing (ChL), Differences between Chemical Leasing and Other Alternative Business Models for Chemicals, Sustainable Chemical Warehousing- Risk Management in the Chemical Warehouse, F<sup>3</sup>-Factory concept, Indian energy security scenarios (IESS) 2047.

#### Unit 2 Process Intensification I

Opportunities and Perspectives for a Sustainable Process Design Definition and Concept, Reaction Engineering, Mixing Principles, Transport Processes, Enhanced Transport Processes, Integrating Process Steps. Moving from Batch to Continuous Processing, Spinning Disc Reactor (Design, Operating Features

and Characteristics of SDRs- Green Synthesis of Nanoparticles using SDR), Micro Process Technology- Transport Intensification, Chemical Intensification, Process Design Intensification. Oscillatory Baffled Reactors- Design and operations. Monolith Reactors for Intensified Processing- Design, Hydrodynamics, Advantages and Applications- Cleaner Production of Fuels and Removal of Toxic Emissions. Cavitational Reactors, Mechanism, Reactor Configurations, Transesterification of Vegetable Oils Using Alcohol using Cavitation

### **Unit 2 Process Intensification II**

Membrane Technology- Definitions, functions and operations, Biocatalytic Membrane Reactors (Entrapment, Gelification and Chemical Attachment), Biofuel Production Using Enzymatic Transesterification. Membrane Technology in Metal Ion Removal from Waste Water, Membrane Operations for the Production of Optically Pure Enantiomers, Integrated Membrane Processes for Water Desalination. Reactive Distillation Technology and Reactive Extraction Technology- Principles, control design and applications. Reactive Absorption Technology in Carbon Dioxide Capture, removal of Nitrogen Oxides, Desulfurization, and in Sulfuric and Nitric Acid production

### **Unit 4 Computer Applications in Catalytic Research**

Computers as research tools in catalysis- a brief overview, a short overview of modelling methods, Data-mining methods in catalysis (PCA, PLS and Artificial Neural networks)

### **Unit 5 Successful Example of Sustainable Industrial Chemistry**

Detailed Process Chemistry of the current technologies and routes for the following chemicals in industry. Industrial Propene Oxide Production (CHPO (Chlorohydrin) Technology, PO/TBA Technology, PO/SM Technology, PO-only Routes). Synthesis of Adipic Acid (Current Technologies for AA Production- Two-Step Transformation of Cyclohexane, Alternatives for AA Production). Ecofining- New Process for Green Diesel Production from Vegetable Oil. Direct Oxidation of Benzene to Phenol, Friedel–Crafts Acylation of Aromatic Ethers Using Zeolites, Sustainable Chemistry in the Production of Nicotines. Homogeneous catalysis: The Shell higher olefin process (SHOP) and Du Pont synthesis of Adiponitrile. Heterogeneous catalysis: The BP AVADA ethyl acetate process

### **Reference**

1. Management Principles of Sustainable Industrial Chemistry, Genserik L.L. Reniers, Kenneth Sorensen, " and Karl Vrancken (Eds), Wiley-VCH Verlag & Co. KGaA, Boschstr. 12, 69469 Weinheim, Germany, 2013
2. Sustainable Development in Practice, Azapagic, A., Perdan, S. (eds.), Wiley-VCH Verlag & Co. KGaA, Boschstr. 12, 69469 Weinheim, Germany, 2011
3. The Art of Process Chemistry, Yasuda, N. (ed.), Wiley-VCH Verlag & Co. KGaA, Boschstr. 12, 69469 Weinheim, Germany, 2011
4. Sustainable Industrial Chemistry, Centi, G., Trifiro, F., Perathoner, S., Cavani, F. (eds.), Wiley-VCH Verlag & Co. KGaA, Boschstr. 12, 69469 Weinheim, Germany, 2009
5. Green chemistry, Fundamentals and Applications, Suresh C. Ameta and Rakshit Ameta, CRC Press, Apple Academic Press, Inc, Taylor & Francis Group, 2013
6. Catalysis: concepts and applications, Gadi Rothenberg, Wiley-VCH Verlag & Co. KGaA, Weinheim, Germany, 2008

**Learning Outcomes:** In this course students learn about sustainable industrial processes, process intensification methods and computer applications in industrial catalysis. This knowledge is essential for the students to seek a profession in chemical industries.

### **Evaluation Pattern – R.13 & R.16**

## Course Outcomes

After completion of the course, a student has

**CO 1:** Ability to engage in safe laboratory practices handling laboratory glassware, equipments, and chemical reagents

**CO 2:** Capacity in predicting the outcome of some simple organic reactions, using a basic understanding of the relative reactivity of functional groups.

## Course Contents:

### 1. Separation of binary mixtures

Includes separation, preliminary investigations, determinations of saturation/unsaturation, detection of elements by Lassaigne's test, functional group identification, derivative preparation, determination of melting points of the derivatives and calculation of  $R_f$  values from TLC

The following mixtures can be given:

- (a) Acid and hydrocarbon
- (b) Phenol and aldehyde
- (c) Phenol and acid
- (d) Phenol and amine
- (e) Acid and ester
- (f) Halo compound and aldehyde
- (g) Acid and aldehyde
- (h) Amine and aldehyde
- (i) Amine and ketone
- (j) Alcohol and hydrocarbon

### 2. Thin layer chromatography to determine $R_f$ values of compounds

- (a) 2-nitroaniline
- (b) 4-nitroaniline
- (c) Cinnamic acid and 2-nitroaniline
- (d) Acetophenone
- (e) Ethyl benzoate

### 3. Simple column chromatography to separate the components of binary mixtures

- (a) Hydrocarbon and ester
- (b) Aldehyde and amine

## REFERENCES:

1. P.W.G. Smith, A.J. Hannaford, B.S.Furnis and A.R. Tatchell, "Vogel's Textbook of Practical Organic Chemistry", ELBS/Longman, 1989.
2. Ralph L. Shriner, Christine K.F. Hermann, Terence C. Morrill, David Y. Curtin, Reynold C. Fuson, 'Systematic Identification of Organic Compounds', John Wiley & Sons, 2003.
3. Mann and Saunders, 'Practical Organic Chemistry', Pearson edition, 2009.

**Learning Outcomes:** After the completion of course students will be able to separate organic binary mixture using ether as solvent and determine whether the components are saturated/unsaturated. They will be able to identify functional groups present in each component, detect the elements present and prepare derivatives of the specific compounds and report the observations in a systematic manner. Qualitative testing of organic compound will be helpful in seeking job to pharma, plastics and R & D in chemical companies.

## Evaluation Pattern – R.13 & R.16

**18CHY682 INSTRUMENTAL METHODS OF ANALYSIS LAB. 0 0 5 2**

### Course Outcomes

The course helps a student to

**CO 1:** Develop skill to analyze the effect of electrochemical parameters for industrial anodisation.

**CO 2:** Acquire the knowledge to apply the principles of electrolyte conductance and electrode potential for analytical applications.

**CO 3:** Attain the skill to evaluate the optical properties of chemical species for analytical applications.

**CO 4:** Understand the rate of electrochemical reactions and applying it for industrial corrosion.

### Course Contents:

1. Determination of strengths of halides in a mixture potentiometrically.
2. To find the redox potential of the given sample using cyclic voltametry.
3. Determination of half wave potential of Cd & Zn by polarography.
4. Determination of pKa of an indicator in aqueous and micellar medium using UV-Vis spectroscopy.
5. Determination of stoichiometry and stability constant of inorganic (ferric-salicylic acid) and organic (amineiodine) complexes using UV-Vis spectroscopy.
6. Determination of copper and cadmium in a mixture by electrogravimetry.
7. Determination of rate constant for enzyme kinetics-inversion of sucrose.
8. Determination of molecular weight of a polymer by Viscometry.
9. Determination of a molecular weight of a solute using Beckmann thermometer.
10. Refractometric determination of composition of solutions.

### TEXTBOOKS:

1. Alexander Findly, 'Practical physical chemistry', 9<sup>th</sup> edition, Wiley, 1972.
2. R.C. Das and B. Behera, 'Experimental Physical Chemistry', Tata McGraw-Hill, 1983.

### REFERENCE BOOKS:

1. J. B. Yadav, 'Advanced Practical Physical Chemisty', Krishna Prakashan Media, 29<sup>th</sup> edition, 2010.
2. Francis William Gray, 'A Manual of Practical Physical Chemistry' Macmillan and Co., Limited, 1914.

**Learning Outcomes:** In this lab course, students learn to use various analytical instruments for the analyses of different paramaters of the chemical compounds. The training they get here is very useful for their further studies with advanced chemistry courses as well as for seeking analytical chemistry related jobs.

## Evaluation Pattern – R.13 & R.16

**18CUL501**

**CULTURAL EDUCATION**

**2 0 0 2**

## Course Contents:

1. Invocation, Satsang and Question - Answers
2. Values - What are they? Definition, Guiding Principles with examples Sharingown experiences
3. Values - Key to meaningful life. Values in different contexts
4. Personality - Mind, Soul and Consciousness - Q and A. Body-Mind-Intellect and the Inner psyche Experience sharing
5. Psychological Significance of samskara (with eg. From Epics)
6. Indian Heritage and Contribution and Q and A; Indian Ethos and Culture
7. Self Discipline (Evolution and Practice) – Q and A
8. Human Development and Spiritual Growth - Q and A
9. Purpose of Life plus Q and A
10. Cultivating self Development
11. Self effort and Divine Grace - their roles – Q and A; - Vedanta and Creation -Understanding a spiritual Master
12. Dimensions of Spiritual Education; Need for change Lecture – 1; Need for Perfection Lecture - 2
13. How to help others who have achieved less - Man and Nature Q and A, Sharing of experiences

## REFERENCES:

1. Swami AmritaswaroopanandaPuri - *Awaken Children (Volume VII and VIII)*
2. Swami AmritaswaroopanandaPuri - *Amma's Heart*
3. Swami RamakrishnandaPuri - *Rising Along the Razor's Edge*
4. Deepak Chopra - *Book 1: Quantum Healing; Book 2: Alpha and Omega of God; Book 3: Seven Spiritual Rules for Success*
5. Dr. A. P. J. Abdul Kalam - *1. Ignited Minds 2. Talks (CD)*
6. Swami RamakrishnandaPuri - *Ultimate Success*
7. Swami JnanamritanandaPuri - *Upadesamritham (Trans: Malayalam)*
8. Vedanta Kesari Publication - *Values - Key to a meaningful life*
9. Swami Ranganathananda - *Eternal values for a changing society*
10. David Megginson and Vivien Whitaker - *Cultivating Self Development*
11. Elizabeth B. Hurlock - *Personality Development, Tata McGraw Hill*
12. Swami Jagatmananda - *Learn to Live (Vol.1 and 2), RK Ashram, Myslapore*

**Learning Outcome:** Love is the substratum of life and spirituality. If love is absent life becomes meaningless. In the present world if love is used as the string to connect the beads of values, life becomes precious, rare and beautiful like a fragrant blossom. Values are not to be learned alone. They have to be imbibed into the inner spirit and put into practice. This should happen at the right time when you have vitality and strength, when your hearts are open. The present course in value education is a humble experience-based effort to lead and metamorphosis the students through the process of transformation of their inner self towards achieving the best. Amma's nectarous words of wisdom and acts of love are our guiding principles. Amma's philosophy provides an insight into the vision of our optimistic future.

## Evaluation Pattern – R.13 & R.16

## OPEN ELECTIVES

18OEL631 ADVANCED STATISTICAL ANALYSIS FOR RESEARCH

2002

## Course Contents:

## **Unit 1**

Relevance of statistical analysis in research – scope of analysis in research - types of research – types of analysis in different areas.

## **Unit 2**

Test of hypothesis - hypothesis testing procedure – significance level – steps for testing.

## **Unit 3**

Chi-Square – t Test.

## **Unit 4**

Tools for statistical analysis – familiarising the tool window – common buttons – available menu – entering and editing data.

## **Unit 5**

Different types of analysis using tool.

### **REFERENCE BOOK:**

*C, R Kothari, Research methodology – Methods and techniques, New Age International Publishers*

**Learning Outcome:** This course familiarizes students with the application of statistical tool to enable them to easily perform complicated quantitative analysis.

## **Evaluation Pattern – R.13 & R.16**

180EL632

**BASICS OF PC SOFTWARE**

**2 0 0 2**

### **Course Contents:**

#### **Unit 1**

Word Processing Basic - An Introduction to Word Processing, Opening Word Processing package, menu bar, Using the help, Using the Icons below menu bar. Opening, saving and closing documents. Page setup, Page background, Printing of documents, Display/Hiding of Paragraph Marks and inter word Space. Moving around in a document - Scrolling the Document, Scrolling by line/paragraph, Fast scrolling and Moving Pages Text creation and manipulation - Paragraph and Tab setting, Text selection, cut, copy and paste, font and size selection, bold, italic and underline, Alignment of text: center, left, right and justify. Formatting the Text - Changing font, size and color, Paragraph indenting, bullets and numbering, Use of tab and Tab setting, changing case. Inserting – header and footer, page number, date & time, symbols, comments, auto texts, footnotes, citations, caption, index, pictures, files & objects, bookmark, hyperlink.

#### **Unit 2**

Handling multiple documents, Opening and closing of multiple documents, cut, copy and paste across the documents. Table Manipulation - Concept of table, rows columns and cells, draw table, changing cell width and height, alignment of text in cell, copying of cell, delete/insertion of row and columns, borders for table. Printing – printing, print preview, print a selected page. Language Utilities – spelling & grammar- Mail merge options, password locking, View – Macros, document views

#### **Unit 3**

Elements of Electronics Spread Sheet, Application/usage of Electronic Spread Sheet, Opening of spreadsheet, and menu bar, Creation of cells and addressing of cells, cell inputting. Insert – tables, charts. Illustrations, links, texts.

Page Layout – Themes, set up, scale, sheet, arrange. Practicing auto formatting and conditional formatting - Spelling and auto correct – Arranging windows – Freeze panes – Hiding windows. Providing Formulas - Using basic functions/ formalism a cell, Sum function, Average, Percentage, Other basic functions Data – connections, sort & filter, data tools, outline

#### **Unit 4**

Inserting slides – new slides, existing slides, duplicate slides, slides from Auto layout. Slide views – normal, slider sorter. Slide layouts, design templates. Deleting slides. Slide show – start with first slide, current slide, customize show. Inserting header & footer, Date and Time, Hyperlink, Format – Font, Bullet & Numbering. Custom animation, slide Transition.

#### **Unit 5**

Internet: Introduction to networks and internet, history, working of Internet, Modes of connecting to internet, ISPs, Internet address, standard address, domain name, Modems.

World Wide Web-Introduction, Miscellaneous Web Browsers details, searching the w w w - Directories search engines and meta search engines, search fundamentals, search engines, working of the search engines, Telnet and FTP.

#### **TEXTBOOK:**

*Alexis Leon & Mathews Leon: Fundamentals of Information Technology, Vikas Publishing*

#### **REFERENCE BOOKS:**

1. *Microsoft Office 2000 Complete, BPB publications*
2. *Dennis P.Curtin, Kim Foley, Kunal Sen, Cathleen Morin: Information Technology - The Breaking Wave, TATA McGraw-Hill Edition*

**Learning Outcomes:** This course familiarizes the basic concepts of MicrosoftOffice 2007to the applications, which promote students to build their knowledge in business applications.

### **Evaluation Pattern – R.13 & R.16**

**18OEL633**

**COMPUTER HARDWARE AND NETWORKING**

**1 0 1**

**2**

#### **Course Contents:**

##### **Unit 1**

Hardware Basics - Basic Terms, Concepts, and Functions of System Modules, Front and rear panel view of system – Motherboards: Components and Architecture. Popular CPU Chips and their Characteristics, Processor Architecture - Processor specifications - installing and uninstalling processor - CPU Overheating issues – common problems and solutions

##### **Unit 2**

Memory and Storage: Memory features – Types of memory – working - Installing and uninstalling memory modules –maintenance and troubleshooting – common problems and solutions. Storage devices – Hard disk details – Working and parts of hard disks – Installing hard disks – maintenance and troubleshooting.

##### **Unit 3**

Power supply – SMPS – features – types – installing SMPS – Specification for SMPS. Maintenance and

Troubleshooting: Preventive Maintenance and Safety Procedures - Managing Replaceable Components.

#### **Unit 4**

Introducing Computer Networks: Overview - Types - Topology - Networks Defined by Resource Location - Client-Server Networks - Peer-to-Peer Networks - Dissecting the OSI Model - The TCP/IP Stack Layers of the TCP/IP Stack - Common Application Protocols in the TCP/IP Stack.

#### **Unit 5**

Networking Devices – Repeater, Hub, Switch, Router – Basics of Types of cabling – Crimping - Setting up a LAN.

#### **TEXT BOOKS / REFERENCE BOOKS**

1. James K L, "Computer Hardware: Installation, Interfacing Troubleshooting and maintenance", PHI Learning Press (Eastern Economy Edition, 2013)
2. Mark Dye, Rick McDonald, Antoon Ruffi, "Network Fundamentals: CCNA Exploration Companion Guide", Cisco Networking Academy, 2008
3. Kaveh Pahlavan, Prashant Krishnamurthy, "Networking Fundamentals: Wide, Local and Personal Area Communications", Paperback, 2014

**Learning Outcome:** This course gives a general understanding of how a computer works. Students will be able to understand the basics of hardware and Networking technologies.

### **Evaluation Pattern – R.13 & R.16**

18OEL634

CONSUMER PROTECTION ACT

2 0 0 2

#### **Course Contents:**

##### **Unit 1**

Consumerism in India (Historical Background), Consumers: the concept, definition and scope. Object of Consumer Protection Act, 1986.

##### **Unit 2**

Unfair Trade Practice, Restriction Trade Practice, Defect in goods, Deficiency in service: Medical, Lawyering, Electricity, Housing, Postal services etc.

**Unit 3** Consumer rights and its protection; consumer protection councils, powers and functions.

**Unit 4** Judicial Enforcement of Consumer Rights: Consumer Forum under C.P.Act -Jurisdiction, Powers and functions, Exceptions of order, Judicial Review, PIL, Class action, Remedies, Appeal, Administrative Remedies, C.P.Courts.

**Unit 5** Appeals and orders: enforcement of orders of the consumer forum, Appeals against orders, Administrative control; Dismissal of frivolous and vexatious complaints, Penalties.

#### **REFERENCE TEXTS:**

1. Saraf D.N., *Law of Consumer Protection in India*, 1995
2. R.K.Bangia, *Consumer Protection Act*
3. P.K.Majumdar, *The Law of Consumer Protection in India*, 1998 Orient Publishing Co. Delhi



**Learning Outcome:** This course gives information about consumer rights and to understand the grievances redressal forums established under the Consumer Protection Act, 1986.

## Evaluation Pattern – R.13 & R.16

18OEL635

CORPORATE COMMUNICATION

2002

### Course Contents:

#### Unit 1

Structure and characteristics of an organization; Factors influencing communication  
Flow of communication in an organization - Bottom up, top down vertical and horizontal barriers to communication; Organization of a PR department and counselling firms.

#### Unit 2

Role of PR in an organization; PR processes - image building - PR and various publics - internal & external; PR and crisis management- national community, labour unrest, and accidents.

#### Unit 3

PR tools - House journals - kinds and production of house journals; Open house; New media; Gossip, rumour mongering and criticism.

#### Unit 4

Media Relations - press conference, press releases, press visit, interviews, preparations and distributions of publicity materials to media.

#### Unit 5

PR for Govt. PR for Non Govt. organizations, PR for armed forces, PR for entertainment and sports, PR for tourism, PR for philanthropic organizations, PR for celebrities. Event management, Ethics in PR.

### **BOOKS RECOMMENDED:**

1. Balan K.R.: *Lectures on applied Public Relations.*
2. Dennis L. Wilcox, Philip H. Ault & Warren K. Agee: *Public Relations strategies & tactics.*
3. Mehta D.S.: *Handbook of Public Relations in India*
4. Scott M. Cutlip, Allen H. Centre & Glen M. Broom: *Effective Public Relations.*
5. Philip Lesley: *Lesley's Public Relations Handbook*
6. Kaul J.M.: *Public Relations Handbook.*
7. Frank Jefkins: *Planned Public Relations*
8. Sam Black: *The role of Public Relations in Management.*

## Evaluation Pattern – R.13 & R.16

18OEL636

DESIGN STUDIES

2002

## **Course Contents:**

### **Unit 1**

Drawing and illustration.

### **Unit 2**

Design basics.

### **Unit 3**

Principles of composition.

### **Unit 4**

Introduction to type design.

### **Unit 5**

Usage of images, colour in terms of visual design.

### **REFERENCES:**

1. *Thinking with Type* by Ellen Lupton

2. *How to be a Graphic Designer Without Losing Your Soul* by Adrian Shaughnessy

**Learning Outcome:** This course introduce the students to the field of visual design.

## **Evaluation Pattern – R.13 & R.16**

18OEL637

**DISASTER MANAGEMENT**

**2 0 0 2**

## **Course Contents:**

**Unit 1** Introduction & Dimensions of Natural & Anthropogenic Disasters, Principles/Components of Disaster Management, Organizational Structure for Disaster Management,

**Unit 2** Disaster Management Schemes/ standard operating procedures, Natural Disasters and Mitigation Efforts, Flood Control, Drought Management, Cyclones, Avalanches, Mangroves, Land Use Planning, Inter-Linking of Rivers, Role of Union/ States, Role of Armed Forces/ Other Agencies In Disasters, Important Statutes/ Legal Provisions, Improvised Explosive Device/ Bomb Threat Planning, Nuclear, biological and chemical threat And Safety Measures, Forest Fires, Oil Fires, Crisis In Power Sector, Accidents In Coal Mines, Terrorism And Emergency Management.

Operations Management (OM), Risk Assessment and Disaster Response, Quantification Techniques, NGO Management, SWOT Analysis based on Design & Formulation Strategies,

**Unit 3** Insurance & Risk Management, Role of Financial Institutions in Mitigation Effort, Group Dynamics, Concept of Team Building, Motivation Theories and Applications, School Awareness and Safety Programmes, Psychological and Social Dimensions in Disasters, Trauma and Stress, Emotional Intelligence, Electronic Warning Systems, Recent Trends in Disaster Information Provider, Geo Informatics in Disaster Studies, Cyber Terrorism, Remote Sensing & GIS Technology, Laser Scanning Applications in Disaster Management, Statistical Seismology, Quick Reconstruction Technologies,

**Unit 4** Role of Media in Disasters, Management of Epidemics, Bio-Terrorism, Forecasting/ Management of Casualties.

**Unit 5** Case Studies - Natural Disaster and Man-made Disasters.

**REFERENCES:**

1. *Disaster Management - Harsh K Gupta*
2. *Disaster Management - Damon.P*

**Learning Outcome:** This course provides the information about the fundamentals of disaster management and introduces the fundamentals procedure and working during the contingency.

**18OEL638**

**ESSENTIALS OF CULTURAL STUDIES**

**2 0 0 2**

**Course Contents:**

Uniqueness of Indian culture.

Real Indian History.

Heritage – spiritual and cultural heritage.

Glory of ancient India – inventions and discoveries in all fields.

Importance of festivals.

**REFERENCE TEXTS:**

- *Swami Harshananda – Hindu Culture*
- *Amma – Eternal Truth*

**Evaluation Pattern – R.13 & R.16**

**18OEL639**

**FOUNDATIONS OF MATHEMATICS**

**2 0 0 2**

**Course Contents:**

**Unit 1**

Matrices: Type of matrices, addition, subtraction, multiplication of matrices, transpose, determinant of a matrix, adjoint and inverse of a matrix.

**Unit 2**

System of equations - Solution of equations in one(linear, quadratic), two and three variables, Solution of a system of linear equation having unique solution and involving not more than three variables by matrix method, Cramer's rule.

**Unit 3**

Financial mathematics: Simple interest and compound interest.

**Unit 4**

Simple differentiation: functions, simple differentiation of algebraic functions, first and second order derivatives, maxima and minima.

## Unit 5

Elementary integral calculus: Integration of simple algebraic functions.

### REFERENCES:

1. P.R Vittal - *Business mathematics and statistics*, Margham Publications, Chennai.
2. Dr. Amarnath Dikshit, Dr. Jinendra Kumar Jain - *Business mathematics*, Himalaya publishing House.
3. V.K Kapoor - *Introductory Business mathematics*, Sultan chand & Sons, New Delhi.

**Learning Outcome:** This course helps to develop an understanding of problem solving methods, to understand the basic concepts of mathematics and to apply the results to real life business problems.

## Evaluation Pattern – R.13 & R.16

18OEL640

FOUNDATIONS OF QUANTUM MECHANICS

2 0 0 2

### Course Contents:

#### Unit 1

Historical Perspective of Quantum Physics: Failure of classical mechanics - Planck-Einstein, Bohr-de Broglie-Heisenberg's Uncertainty.

#### Unit 2

Empirical confirmations of Wave Particle Duality. Schrödinger Equation - Particle in a box-Tunnel effect.

#### Unit 3

Paradoxes in QM - de Broglie paradox - Schrödinger's cat, Mach-Zehnder type interferometers - EPR paradox - Bell-type Inequalities.

#### Unit 4

Various interpretations - Statistical, Copenhagen, Bohm's formulation, Transactional, Wheeler's Participatory Universe, Many World, Decoherence, consciousness interpretation.

#### Unit 5

Uncertainty-Nonlocality, Holistic universe, Violations of causality-Retro influence-Philosophy of Advaita (non-Duality).

### TEXT AND REFERENCES:

1. *Quantum Enigma: Physics Encounters Consciousness* by Bruce Rosenblum and Fred Kuttner (Aug 1, 2011)
2. *The New Physics and Cosmology* Zanjoc, Oxford 2004

## Evaluation Pattern – R.13 & R.16

18OEL641  
LITERATURE

GLIMPSES OF LIFE THROUGH

2 0 0 2

## **Course Contents:**

### **Unit 1**

- 1 Introduction – What literature is – Language and literature – Indian literature – Values through literature – Literature and culture – Enjoying literature
- 2 Father Giligan – WB Yeats

### **Unit 2**

- 3 The West Wind – PB Shelley
- 4 Chicago Address – Swami Vivekananda

### **Unit 3**

- 5 On Saying Please – AG Gardiner
- 6 My Lost Dollar – Stephen Leacock
- 7 The Importance of Being Earnest – Oscar Wilde (extracts)

### **Unit 4**

- 8 The Refugee – AK Abbas
- 9 The Mirrored Hall – Swami Chinmayananda

### **Unit 5**

- 10 The Windhover – GM Hopkins

## **Evaluation Pattern – R.13 & R.16**

**18OEL642**

**INFORMATION TECHNOLOGY IN BANKING**

**2 0 0 2**

## **Course Contents:**

### **Unit 1**

Bank and Banking: Meaning and definition, development of banking in India, types banks, banking systems, types of banking systems, commercial banks, functions, nationalization of commercial banks in India.

### **Unit 2**

Central Banking, functions, Reserve Bank of India, State Bank of India.

### **Unit 3**

Banker and Customer, opening an account, Pass Book and Pay-in Slip, Cheques, types of cheques, crossing of cheques.

### **Unit 4**

Role of information technology in banking services, Core Banking, Automated Teller Machine (ATM), Electronic Clearing Service (ECS), NEFT and RTGS, Mobile Banking.

### **Unit 5**

Debit Card and Credit Card, banking and E-Commerce, Point of Sales (PoS), Online bill payment and ticket reservation – future of electronic banking.

## **REFERENCE BOOKS:**

1. Sundaram and Varshney – *Banking Law, Theory and Practice*, Sultan Chand
2. B. Santhanam – *Banking and Financial Systems*, Margham Publications
3. S.N. Maheswari – *Banking Law, Theory and Practice*, Kalyani Publications
4. Parameswaran – *Indian Banking*, S.Chand and Co

**Learning Outcome:** This course provides an understanding on the technology enabled banking services and their applications.

## Evaluation Pattern – R.13 & R.16

18OEL643

INTRODUCTION TO WEB TECHNOLOGIES

2002

### Course Contents:

#### Unit 1

Internet Basics: Introduction to Internet, Communications on Internet, Resources of Internet – H/w and s/w requirements of Internet – ISP – Choosing an ISP – Internet Domains - Internet Applications – WWW - FTP, Telnet.

#### Unit 2

Introduction to HTML: HTML Tags, Paired Tags, Singular Tags, Commonly Used HTML commands, DOCTYPE Element, The HTML element, The HEAD Element, BODY, TITLE and Footers, Layout HTML Tags, Formatting Tags, Text Formatting and style Formatting, Effects, Spacing, Bullets and Numbering, Ordered lists, Unordered Lists, Definition Lists, HyperLink, Working with Images.

Style Sheet: The CSS standards, Types, Introducing CSS, Applying styles to specific groups of elements, Font Attributes, Color and Background attributes, Text Attributes Border, Margin, Using the Class name Style Sheet Selector, Using the ID style sheet Selector, Inline Styles, linking External Style Sheets.

Tables for Organization and Layout The basic table Elements, Column grouping with COLGROUP & COL, Row grouping, Table Caption.

#### Unit 3

Forms and Form Elements: What are HTML forms, The FORM Object and its Attributes, The Form Elements, The Button Element, Creating a Selection List, Adding radio buttons and Check boxes to a Web page, Accessing Text with the Text controls: text, textarea, and password, Submitting and Resetting the Form with submit and reset.

Frames and Frameset: Creating and Working with Frames, The FRAMESET Element, Nested Framesets, The Frame Element, Accessing external references from Frame, Inline Frames with IFRAME.

#### Unit 4

Scripting Basics: What is Client, Side scripting, Scripts and Programs, Introduction to JavaScript syntax, Statements, Blocks, Comments, Data Types, String, Numbers, Boolean Variable, Expressions, Numerical and Logical Expressions, Flow Control, Creating Simple JavaScript.

#### Unit 5

Introduction to E-commerce: E-commerce consumer applications, E-commerce organization applications, Consumer Oriented applications, Mercantile process models, Consumer's perspective of Mercantile process models, Merchant's perspective of Mercantile process model.

## **TEXTBOOKS**

1. Ivan Bayross, *Web Enabled Commercial Application Development Using HTML, JavaScript, DHTML and PHP, 4th Revised Edition, BPB Publications*
2. Henry Chan, Raymond Lee, Tharam Dillon, Elizabeth Chang, *E-Commerce and Applications, Wiley Publications*

**Learning Outcome:** This course gives an overview about developing attractive web sites and basic concepts of e-commerce.

## **Evaluation Pattern – R.13 & R.16**

18OEL644

KNOWLEDGE MANAGEMENT

2 0 0 2

### **Course Contents:**

#### **Unit 1**

Knowledge management concepts – Introduction - Definitions of Knowledge – Data-information and knowledge - basic thoughts on knowledge - difference between wisdom and knowledge - information Management and knowledge Management - hierarchy model - knowledge types – explicitness – reach - abstraction level – propositionality – Earl’s schools of knowledge management.

#### **Unit 2**

Knowledge management and process - Becerra-Fernandez and Stevenson knowledge process - Nonaka’s Knowledge Spiral – dynamics of knowledge creation – knowledge management systems – knowledge management sub – processes – knowledge discovery – knowledge capture – knowledge sharing –knowledge application.

#### **Unit 3**

Organizational knowledge – Need – benefits - components and functions - Knowledge management in virtual organizations - knowledge management in professions - a study of IT and ITES business - knowledge management system requirements - Organizational knowledge measurement techniques - organizational implementation barriers.

#### **Unit 4**

Designing Enterprise Knowledge Management System architecture – Multi-layer architecture for Knowledge Management Systems - knowledge management in decentralized and heterogeneous corporations - Web based knowledge management support for document collections.

#### **Unit 5**

Recent Tools for KM - Intelligent support systems - intelligent systems and artificial intelligence - comparing artificial and neural intelligence - conventional vs. Artificial intelligence - Emerging technology - virtual reality - Intellectual capital.

### **TEXTBOOKS AND REFERENCES:**

1. *Knowledge Management – Sudhir Warier, Vikas Publications.*
2. *Knowledge Management Systems – Stuart Barnes, Thomson Learning.*
3. *Key issues in the New Knowledge Management – J.M. Firestone, M.W. Mcelroy.*
4. *Developing Expert System for Business – Chandler/Liang.*

**Learning Outcome:** This course enables students to understand the basics of Knowledge Management and its applications in organizations.

## Evaluation Pattern – R.13 & R.16

18OEL645

MARKETING RESEARCH

2 0 0 2

### Course Contents:

#### Unit 1

Definition of Marketing Research, Objective of Marketing Research, Application of Marketing Research, Limitation of Marketing Research, Marketing Research Process.

#### Unit 2

Research Design: Various Method of Research Design, Important Experimental Research Designs.

Primary and Secondary Data: Methods of Collecting Primary Data, Advantages & Disadvantages of Primary Data & Secondary Data, Essentials Characteristics for Selecting Secondary Data. Basic Methods of Collecting Data: Questionnaire Method/ Observation Method - Advantages & Disadvantages, Methods of Observation, Precautions in Preparation of Questionnaire & Collection of Data.

#### Unit 3

Measurement and Scaling: Types of Scales, Difficulty of Measurement, Sources of Error, Criteria for a Good Scale, Development of Marketing Measures.

Sampling: What is Sampling, Objective of Sampling, Steps in Sample Design, Various Techniques of Sampling, Advantages & Disadvantages of Different Techniques of Sampling, Difference between Probability and Non-probability Sampling, Problem Associated with Sampling, Determining Sample Size.

#### Unit 4

Data Processing, Analysis and Estimation

#### Unit 5

Report Preparation: Types and Layout of Research Report; Precautions in Preparing the Research Report, Bibliography and Annexure in Report, Drawing Conclusions, Giving Suggestions and Recommendation to the Concerned Persons.

### REFERENCE TEXTS:

1. Nargundkar - Marketing Research, Tata McGraw Hill, 2nd Ed.
2. Luck and Rubin - Marketing Research, Prentice Hall of India, 7th Ed.
3. Tull & Hawkins - Marketing Research: Measurement & Method, Prentice Hall of India, 6th Ed.
4. Beri - Marketing Research, Tata McGraw Hill, 4th Ed.

**Learning Outcome:** This course provides a basic knowledge on research methodology and market research.



## Evaluation Pattern – R.13 & R.16

18OEL646

MEDIA FOR SOCIAL CHANGE

2 0 0 2

### Course Contents:

#### Unit 1 Health Communication

Introduction to theories in Health Communication. Awareness on Health Issues – Epidemic Diseases, knowledge about vaccination for various diseases - Health campaign will be organized with the help of Medical Practitioner.

#### Unit 2 Radio for Social Change

Awareness on Edaphic Issues - Soil Pollution, Water Pollution and other forms of pollution. Anti-Pollution campaign will be organized with the help of Environmental Scientist or Journalist.

#### Unit 3 Social Media Activism

Awareness on Blood Donation – How a tiny red drop makes someone's life Green. Awareness campaign will be organized based on Eye Donation.

#### Unit 4 Development Communication and Social Learning

Locating the remote village where basic amenities like Water, Toilet facilities are not available - A campaign with the involvement of government officials and social scientists.

#### Unit 5 Participatory Communication for Social Change

Organic Farming - Awareness of Organic Farming. Benefits of organic farming in the materialistic world. A campaign cum workshop will be conducted by inviting experts from Agricultural Husbandry.

### REFERENCES

1. *Tillman, C. (2006). Principles of occupational health and hygiene: an introduction. Allen & Unwin.*
2. *Thayer, Lee, (2014) Mental Hygiene: Communication and the Health of the Mind.*
3. *Harrison, R. M. (2001). Pollution: causes, effects and control. Royal Society of Chemistry. Wilhelm, J. (2016). Environment and Pollution in Colonial India: Sewerage Technologies Along the Sacred Ganges. Routledge.*
4. *Charbonneau, J., & Smith, A. (Eds.). (2015). Giving Blood: The Institutional Making of Altruism. Routledge.*
5. *Agarwal, Arun K (2007) Standard Operating Procedures(sop) For Hospitals In India. New Delhi: Atlantic Publishers*
6. *Atlantic Publishers*
7. *Hall-Matthews, D. N. J. (2005). Peasants, Famine and the State in Colonial Western India.*
8. *Basingstoke: Palgrave Macmillan.*
9. *Thottathil, S. E. (2014). India's Organic Farming Revolution: What it Means for Our Global Food System. University of Iowa Press.*

## Evaluation Pattern – R.13 & R.16

18OEL647

MEDIA MANAGEMENT

2 0 0 2

### Course Contents:

## **Unit 1**

Management concept – Principles of Management - Factors influencing Management decision in media – Structure and characteristics of media organizations – Newspapers and Magazines, Radio, Television, Cinema - Ownership in Media Industries – Merits and de-merits.

## **Unit 2**

Economics of newspaper – Advertising vs circulation – Management problems of small, medium, large newspapers: gathering, processing, printing, circulation, distribution, advertising, professionalism, trade unionism, News room diversity.

## **Unit 3**

Economics and Administrative concerns of government owned electronic media-market driven media: private channels – Social commitment vs Profit making.

## **Unit 4**

Economics of film Industry – creativity, production, marketing distribution, exhibition, ownership vs piracy.

## **Unit 5**

News agencies and syndicates: Ownership and organization structures – committees to study the problems of various media in India.

### **BOOKS RECOMMENDED:**

1. Aggarwal S.K : *Press at the crossroads in India.*
2. William and Rucker: *Newspaper Organization and Management*
3. Sarkar R.C: *The press in India*
4. Noorani A.G: *Freedom of Press in India*
5. Frank Thayer: *Newspaper Management*
6. Gulab Kothari: *Newspaper Management in India*
7. *Reports of the enquiry committees appointed by the Ministry of Information and Broadcasting.*

## **Evaluation Pattern – R.13 & R.16**

18OEL648

**OBJECT-ORIENTED PROGRAMMING**

2 0 0 2

### **Course Contents:**

#### **Unit 1**

Introduction to OOPS: Object Oriented Programming features, Applications, History, Difference from structured Programming, Object Oriented Programming Languages, Program execution.

#### **Unit 2**

Object Oriented Concepts: Abstraction, Encapsulation, Polymorphism, Inheritance, Classes and Objects, Programming Basics - Data types, Conditional Statements, Loops, arrays, Functions, Structures.

#### **Unit 3**

Implementing Class, Object Data Types, User Defined Data Types, Defining a Class, e Access specifiers, The Scope Resolution Operator, Using Class Objects Like Built-in Types, Scope, Constructors, Member Initialization, Constructor Overloading, Destructors.

#### Unit 4

Inheritance: Introduction, The protected Access Level, Assignments Between Base and Derived Objects, Types of Inheritance, Compile-Time vs. Run-Time Binding, virtual Functions, Polymorphism, Abstract Base Classes.

#### Unit 5

The iostream Library, Predefined Streams, Stream States, Formatted I/O, Disk Files, Reading and Writing Objects.

#### TEXTBOOKS

1. E Balaguruswamy “Object Oriented Programming Using C++” 6th Edition, TMH Publications
2. Lalit Kishore Arora , Dr. Vikesh Kumar, “ Object Oriented Programming Using C++ “,S.K. Kataria & Sons; 2011 edition (2011)

### Evaluation Pattern – R.13 & R.16

18OEL649

PAINTING AND SCULPTURE

1 0 1 2

#### Course Contents:

##### Unit 1

Pencil drawing, life study.

##### Unit 2

Basics of water colour painting, Clay modelling.

##### Unit 3

Anatomy and figure study, Basics of oil and acrylic painting.

##### Unit 4

Basics of Figure modeling.

##### Unit 5

Moulding and casting.

#### REFERENCE BOOKS

1. *Indian Sculpture and Painting* – by E.B. Havell (Author)
2. *Modern Painting And Sculpture: 1880 To Present From The Museum Of Modern Art* – by John Elderfield (Editor)

**Learning Outcome:** This course makes students to develop critical thinking skill as well as make them creative in theirfield of painting and sculpture.

### Evaluation Pattern – R.13 & R.16

18OEL650

PERSONAL FINANCE

2 0 0 2

#### Course Contents:

##### Unit 1

Basics of Personal Financial Planning, Time Value of Money, Planning tax strategies.

## **Unit 2**

Introduction to Consumer Credit, sources of credit, Consumer Purchasing, strategies for housing decisions.

## **Unit 3**

Insurance: types, selecting the right insurance policy, property and motor vehicle insurance, health insurance policies, Retirement Planning, NPS.

## **Unit 4**

Investing fundamentals, investing in shares, bonds and mutual funds, investment in gold and real estate.

## **Unit 5**

Investing in Schemes of Government: National Savings Certificates, KVP, Post Office Recurring Deposits and term deposits, PPF.

### **REFERENCE TEXTS:**

1. *Jeff Madura – Personal Finance, Pearson Education*
2. *Manish Chauhan – 16 Personal Finance Principles every Investor should know, Network18 Publishers*
3. *Jack R Kapoor, Les R Dlabey – Personal Finance, McGraw Hill*

**Learning Outcome:** This course helps the students to analyse the process of making personal financial decisions, develop personal financial goals and identify the strategies for their achievement.

## **Evaluation Pattern – R.13 & R.16**

18OEL651

PRINCIPLES OF ADVERTISING

2002

### **Course Contents:**

#### **Unit 1 Introduction**

History of advertising, Advertising-meaning and definition, Advertising as a tool of communication, Features of advertising.

#### **Unit 2 Types of Media – Advantages & Disadvantages**

Types of advertising, Types of media in advertising – Features – advantages – disadvantages – Print, Television, Radio, Internet, OOH.

#### **Unit 3 Structure of an Advertising Agency**

Structure of advertising agency – Small, Medium, National, In-house.

#### **Unit 4 Other Promotion**

Sales Promotion, Direct Marketing, Public Relations, Publicity and Corporate Advertising, Unconventional Promotional Media.

#### **Unit 5 Case Studies**

### **REFERENCE BOOKS:**

1. *Advertising, Frank Jefkins Revised by Daniel Yadin*
2. *Kleppner's Advertising Procedure*

**Learning Outcome:** This course help sstudents to make basic understanding onadvertising, providing understanding on the processes behind successful advertising. The students are introduced to the processes, tools and techniques used in developing advertising concepts with the study areas including creative thinking and visualizing.

## Evaluation Pattern – R.13 & R.16

18OEL652

PRINCIPLES OF PACKAGING

2 0 0 2

### Course Contents:

#### Unit 1

Packaging: Meaning and importance, functions, marketing considerations of packaging.

#### Unit 2

Design of package, materials used for packaging, selection criteria of packaging materials, packing techniques.

#### Unit 3

Packaging systems, future of packaging.

#### Unit 4

Provisions of the Legal Metrology (Packaged Commodities) Rules 2011.

#### Unit 5

Provisions of Food Safety Standards (Packaging and Labelling) Regulations, 2011.

### **REFERENCE TEXTS:**

1. Gordon Robertson – *Food Packaging: Principles and Practice*, CRC Press
2. Frank Paine – *A Handbook of Food Packaging*, Springer

**Learning Outcome:** This course helps the students to analyse the process of making personal financial decisions, develop personal financial goals and identify the strategies for their achievement.

## Evaluation Pattern – R.13 & R.16

18OEL653

SCRIPTING FOR RURAL BROADCASTING

1 0 1 2

### Course Contents:

#### Unit 1

Introduction to rural broadcasting. Rural life and issues. Cultural ecology - Anthropological approaches - traditional social activities-translocal ruralistic features. Practical: Visit any rural area for making detail analysis on the topics during weekends.

#### Unit 2

Rural communities. Analysis of social and political life in a rural community. Caste / class dynamics and regional influences.

#### Unit 3

Scope and Impact of broadcast journalism in rural development. Two day workshop by an external expert from the

broadcast industry on the rudiments of script writing focusing on rural aspects/ communities.

#### **Unit 4**

Practice on Scripting. Focus on covering special issues concerning rural women, youth, farmers, self-help groups cottage industries etc.

#### **Unit 5**

Developing the final script for rural broadcasting that will have practical application in the field. Final evaluation by the external expert.

#### **REFERENCES**

1. Eschenbach, J. (1977). *The role of broadcasting in rural communication*.
2. Friedrich-Ebert-Stiftung. George, A. M. (2004). *India untouched: The forgotten face of rural poverty*. East West Books.
3. Kumar, K. (2003). *Mixed signals: Radio broadcasting policy in India*. *Economic and political weekly*, 2173-2182.
4. Maddison, J. (1971). *Radio and television in literacy*. Unesco.
5. Manyozo, L. (2011). *People's radio: communicating change across Africa*. Southbound Penang
6. Neurath, P. M. (1962). *Radio farm forum as a tool of change in Indian villages*. *Economic Development and Cultural Change*, 10(3), 275-283.
7. Onabajo, F. (2003). *37 Message Design & the Appropriateness of Language in Rural Broadcasting*. *Four Decades in the Study of Languages & Linguistics in Nigeria: O'Hare, K. (1992). Scripts: Writing for Radio and Television*. *Canadian Journal of Communication*, 17(4).
8. Sharma, A., & Kashyap, S. K. (2013). *Information need assessment for empowering rural women through community radio programmes: A study in Tarai region of Uttarakhand*. *Journal of Community Mobilization and Sustainable Development*, 8(2), 169-173.
9. *Community Mobilization and Sustainable Development*, 8(2), 169-173.

### **Evaluation Pattern – R.13 & R.16**

18OEL654

**SOCIAL MEDIA WEBSITE AWARENESS**

1 0 1 2

#### **Course Contents:**

##### **Unit 1**

Introduction to Social media; Definition - Social Media and Digital transformation; Social Networking and online communities; Social support and service; Wikipedia, Facebook, Instagram, Tagging, LinkedIn; Social mobile applications; Security settings in Facebook, Whatsapp.

##### **Unit 2**

Blogging – History; Creating blog, effect of blogging, micro blogging; Protocol, Platform, Content strategies.

##### **Unit 3**

Tweeting - Introduction, History, Protocol; Twitter; Twitter apps; Managing Twitter; #hashtag# creation and following; Security settings in Twitter.

##### **Unit 4**

Social media sharing – History, Protocol; YouTube, Flickr, Slide share, Social news; News apps – Newshunt and others; Bookmarking - History, Digg, Reddit, Delicious.

### **Unit 5**

Social theory in the information age; Social Network for professional, business, Digital Marketing; Using social networking sites for research, Security aspects of social networking.

### **REFERENCES:**

1. *Social Networking - Digital and Information Literacy Series* by Peter K. Ryan, The Rosen Publishing Group, 2011  
ISBN 1448823463, 9781448823468
2. *The Social Media Marketing Book* Dan Zarrella "O'Reilly Media, Inc.", 13-Nov-2009

**Learning Outcome:** This course helps the students to understand the history, theory, technology and uses of social media; to create, collaborate, and share messages with audiences of all sizes; to know and explore the possibilities and limitations of social media. Hands on experience with several forms of social media technology; to understand and use social media productively and to evaluating new tools and platforms.

## **Evaluation Pattern – R.13 & R.16**

**18OEL655**

**THEATRE STUDIES**

**1 0 1 2**

### **Course Contents:**

#### **Unit 1**

Breathing exercises, warming up exercises.

#### **Unit 2**

Voice modulation, Monologue practice.

#### **Unit 3**

Facial expressions, emoting a character.

#### **Unit 4**

Stage direction, Makeup and costumes.

#### **Unit 5**

Choreography, Producing a play.

### **REFERENCES:**

1. *Theatre as Sign System: A Semiotics of Text and Performance* by Elaine Aston, George Savona
2. *Theatre Semiotics: Text and Staging in Modern Theatre* by Fernando de Toro
3. *Acting For Real: Drama Therapy Process, Technique, and Performance* by Renee Emunah

**Learning Outcome:** This course provides students with a firm grounding in the discipline of Theatre and Performance Studies.

## **Evaluation Pattern – R.13 & R.16**

**Course Contents:****Unit 1**

What is Technical Writing? - Purpose and characteristics of technical writing and need for developing technical writing skill. Use of Technical terms, Defining terms, Style and tone.

**Unit 2**

Use of resources, documentation style and citation; Standard operation procedures, Instruction Manuals and Handbooks.

**Unit 3**

Oral presentations, Analysis of published papers – format, content and style.

**Unit 4**

Drafting a research paper for publication; Grammar check and editing; proof reading.

**Unit 5**

Submission of term paper.

**REFERENCE BOOKS:**

1. McMurrey David, *Technical Writing*,
2. Manser Martin H. *Guide to Style: an essential guide to the basics of writing style*, Viva books

**Learning Outcome:** This course familiarizes the students with the requirements of effective technical writing; to enable students to independently work on their publication and presentation of papers; developing skills required for presentation of reports, papers and proposals.

**Evaluation Pattern – R.13 & R.16****Course Contents:****Unit 1**

Yoga and Modern Life – Introduction - understanding Yoga – definition - four streams of yoga - Why yoga?

**Unit 2**

Breath – The Bridge – Introduction - Breathing Practices – Standing - Sitting – Supine.

**Unit 3**

Loosen Yourself – Introduction – Jogging – Bends - Twisting – Pavanamuktasana Kriya.

**Unit 4**

Asanas – Suryanamaskar - Standing Posture - Sitting postures - Prone Postures - Supine – Topsy Turvy - Relaxation



techniques.

### **Unit 5**

Pranayama, Meditation.

#### **REFERENCE TEXTS:**

1. *N.S. Ravishankar – Yoga for Health, Pustak Mahal*
2. *BKS Iyengar – Yoga: The Path to Holistic Health, DK Publishers*

**Learning Outcome:** This course gives an understanding on the concept and advantages of yoga and simple yogapractices.

## **Evaluation Pattern – R.13 & R.16**

18OEL658

FUNDAMENALS OF LEGAL AWARENESS

2002

### **Course Contents:**

#### **Unit 1**

Law and classification: definition, meaning, functions, classification- public and private law, civil law and criminal law, substantive and procedural law, municipal and international law, written and unwritten laws

#### **Unit 2**

Law of contracts: overview of Indian Contract Act, definition, meaning, essentials-offer and acceptance, invitation to offer, cross offers, intention to create legal obligation, lawful consideration, lawful object, competency of parties, free consent, agreement not to be void, illegal, immoral or opposed to public policy, agreement v. contract, breach and remedies for breach.

#### **Unit 3**

Law of torts: Definition, meaning, essentials, damages- injuria sine damnum and damnum sine injuria, general defences in torts, exceptions to tortious liability: vicarious liability- master servant relationship, Principal- agent relationship, Partner- partnership firm, Major torts: Nuisance, Negligence

Tress pass: Tresspass to a person- Battery, Assault, False Imprisonment, defamation- libel and slander, essentials, defences to defamation, liability in torts- strict liability, absolute liability, damages in torts- meaning, types of damages- nominal, compensatory, exemplary, aggravated, prospective, contemptuous

#### **Unit 4**

Criminal law: introduction of criminal law- subject matter, General introduction to the Indian Penal Code, Criminal Procedure code, Indian Evidence Act, mental element- stages of crime, guilty intention, General exceptions- Intoxication, Insanity, Mistake of Fact, Accident, Acts done under compulsion, public duty etc., Right of Private Defence, Major offences: Theft, Extortion, Robbery, Dacoity, Sedition, Abduction, Kidnapping, Unlawful Assembly, Dowry Death, Abetment, Murder, Culpable Homicide

#### **Unit 5**

Family law: subject matter and Introduction, Laws Involved, Marriage – validity and degree of prohibited relationship, Divorce Family Court, Grounds for divorce, orders- judicial separation, restitution of conjugal rights, maintenance, Section 125 Criminal Procedure code, Adoption- difference between guardianship and adoption, General outline of Hindu Adoption and Maintenance Act, Guardianship and Wards Act, Succession- Testamentary and Intestate- Testator, Executor, Administrator and Probate

**Learning Outcome:** This course gives the student the power to make a difference in personal and professional life

through sound legal knowledge and to be aware of rights and responsibilities towards society and nation.

## Evaluation Pattern – R.13 & R.16

18OEL659

SOLID WASTE MANAGEMENT AND UTILIZATION

2 0 0 2

### Course Contents:

#### Unit 1 Biowaste Utilization

Biowaste - Biopesticide from solid waste, biomass to bioethanol, biowaste as carbon source, Bio-digester - generation of renewable energy, biogas from animal waste-daily consumption, Equipment sizing and design.

#### Unit 2 Polymer wastes

Recycling plastic fibre and packaging waste – methods of recycling – Recycling of rubber – Devulcanisation - thermal, mechanical and microbial process - characterization of devulcanized rubber - products from rubber waste. Pyrolysis of plastics and rubber - Catalytic treatment - plastic waste to fuel, oil and wax.

#### Unit 3 Recycling utilized Products

Paper recycling - types of paper, Mechanical and chemical re-pulping, Glass waste-bottle recycling, cullet recycling, process in glass recycling Metals-Iron & steel, iron & steel remanufacturing, Aluminium remanufacturing

#### Unit 4 e-waste

Electronic wastes – printed circuit board, monitors, appliances and batteries, Processing of e-waste, Recovery of heavy metals from electronic waste.

#### Unit 5 Biomedical Waste

Biomedical waste and its category, Treatment-autoclaving, shredding, deep burial & chemical treatment of biomedical waste.

#### REFERENCES:

1. Thomas H. Christensen, *Solid Waste Technology & Management, Vol.1, Blackwell Publishing Ltd, 2011.*
2. Elena Cristina Rada, *Biological Treatment Of Solid Waste, CRC press, 2016.*
3. Martin Forrest, *Recycling and Re-use of Waste Rubber, Smithers Rapra Technology Ltd, 2014.*
4. John Scheirs and Walter Kaminsky, *Feedstock Recycling and Pyrolysis of Waste Plastics, John Wiley & Sons Ltd, 2006.*
5. Ramesha Chandrappa, Diganta Bhusan Das, *Solid Waste Management: Principles and Practice, Springer, 2012.*
6. Hugo Marcelo Veit, Andréa Moura, *Electronic Waste: Recycling Techniques, Springer, 2015.*
7. Lifeng Zhang, Gregory K. Krumdick, *Recycling of Electronic Waste II: Proceedings of the Second Symposium, John Wiley & Sons, Inc, 2011.*

## Evaluation Pattern – R.13 & R.16

18OEL660

RELATIVISTIC QUANTUM MECHANICS

2 0 0 2

### Course Contents:

#### Unit 1 Classical Fields

Particle and Fields, Discrete and Mechanical system, Classical scalar fields, Classical Maxwell fields, Vector potential in quantum mechanics.

#### Unit 2 The quantum theory of radiation

Classical radiation field, Creation, annihilation and number operators, Quantized radiation field, Emission and absorption of photons by atoms

### **Unit 3 Application of quantum theory of radiation**

Rayleigh scattering, Thompson scattering and Raman effect, Radiation damping, Dispersion relations, Lamb shift

### **Unit 4 Relativistic Quantum Mechanics for spin 1/2 particles**

Probability conservation, Dirac equation, Relativistic covariance, Bilinear covariants, Dirac operators in Heisenberg representation, Negative energy solutions

### **Unit 5 Many Particle system**

The hydrogen atom, Hole theory and charge conjugation, Quantization of Dirac field, Weak interaction and non-conservation of parity

#### **TEXTBOOK:**

*Advanced Quantum Mechanics by J. J. Sakurai*

## **Evaluation Pattern – R.13 & R.16**

18OEL661

ROBOTICS AND BIOLOGY

2 0 0 2

#### **Course Contents:**

##### **Unit 1**

Basics of Robotics - Perception, Learning, Terminology, Asimov's Laws of robotics, Robotic Control Loop, Sense-Think-Act components, Types of Robotics

##### **Unit 2**

Evolution, Robot components, Basic electronics, Introduction to mathematical Modeling, Simple models, Logistic growth model and Learning functions.

##### **Unit 3**

Data integration, Biological data, Data fitting, From sources to data-driven modelling, BEAM bots, Kinematics and Movement.

##### **Unit 4**

Applied Psychology, Models of Mind, Control Kinematics, Bio-inspired control, Virtual Bio-inspired robotics lab case studies

##### **Unit 5**

Simple modelling of neuronal robots, Basics of swimming and flying bots, Biomimetic robots, Animal cells and circuits as robotic data devices.

#### **References:**

*Owen Bishop (2007), Robot builder's cookbook, Newnes.*

*Karl Williams (2003), Insectronics, McGraw Hill.*

*Ed. Kato N, Kanimura S (2008), Bio-mechanics of swimming and flying - fluid mechanics, biomimetic robots and sports science, Springer*

## **Evaluation Pattern – R.13 & R.16**

18OEL662

SCIENCE OF WELL-BEING

2 0 0 2

#### **Course Contents:**

## **Unit 1**

Positive Psychology - Happiness, Measuring Happiness, Approaches to Happiness, Benefits of Happiness, Authentic Happiness, Subjective Well-being, Character Strengths, Positive Emotions

## **Unit 2**

Power of Connections - Social Connections and Happiness, Wired for Connection, Affiliation, Affection and Attachment, Family, Parenting, Friends, Active Listening and Empathy

## **Unit 3**

Kindness and Compassion - Altruism, Random Act of Kindness, Evolved for Kindness, Scaling up kindness: contagious kindness, elevation, and heroism

## **Unit 4**

Co-operation and Reconciliation - Peace-making, Forgiveness, Gratitude, Trust

## **Unit 5**

Mindfulness- Attention, Focus, Mindfulness Exercise, Benefits of Mindfulness, Importance of Flow State

### **References:**

*C.R. Snyder & Shane J. Lopez (2009). Oxford Book of Positive Psychology. Oxford University Press.*

*Michael F. Steger (2009). Meaning in Life. The Oxford Handbook of Positive Psychology (2 ed.) Edited by Shane J. Lopez and C.R. Snyder*

*Ronaig D. Seigel (2014). The Science of Mindfulness - A Research - Based path to Well-being. The Great Courses, Virginia*

*Kelly McGonigal (2016). The Science of Compassion: A Modern Approach for Cultivating Empathy, Love, and Connection. Sounds True Publication*

## **Evaluation Pattern – R.13 & R.16**

**18OEL663**

**OPERATING SYSTEMS AND NETWORKS**

**2 0 0 2**

### **Course Contents:**

#### **Unit 1: Introduction to Digital Computer**

Functions and Block Diagram of Computer - Types of Software – System software / Application software / Utility Software - Compilers - Interpreters - Assemblers - Linker - Loader - Programming Language Paradigm.

#### **Unit 2: Data Representation and Memory System**

Binary, Octal, HEX and their inter-conversion - Memory Hierarchy Primary Memory – DRAM, SDRAM, DDR, RDRAM. ROM, PROM, EPROM, EEPROM Concepts of Auxiliary, Associative, Cache and Virtual Memory.

#### **Unit 3: Operating Systems**

Introduction to Operating System – Storage Management: Real Storage Management Strategies – The LINUX Operating - System - Managing Files and Directories – Directory Commands in LINUX – File Commands in LINUX - Securing files in LINUX - File access permissions – viewing File access permissions – Changing File access permissions.

#### **Unit 4: Introduction to communications and Networking**

Introduction – Fundamental concepts - Data communications – Protocols- standards - Analog and Digital signals- Bandwidth of a signal and a medium - The data transmission rate and the bandwidth - Network topologies, switching and routing algorithms: Introduction - Mesh topology - Star topology - Tree topology - Ring topology - Bus topology - Hybrid topology - Switching basics- Circuit switching – Packet switching - Message switching.

#### **Unit 5: Internet and Web Technologies**

Basics of Internet communication - Hardware elements associated with internet - Internet Services - Internet Protocols - TCP/IP, UDP, HTTP - Mail and its types - FTP - Remote access and Transaction - Web Indexes – Search Engines.

Introduction to HTML - Tags and Documents - Link documents using Anchor Tags - Images and Pictures - Tables - HTML Forms - Frames - Framesets - Introduction to Dynamic web applications - Introduction to PHP.

**TEXTBOOKS:**

1. *Operating Systems 2nd Edition.*, H.M. Deitel, Perason, 2003.
2. *Operating System LINUX*, NIIT, PHI, 2006.
3. *Computer Networks – Protocols, Standards and Interfaces*, Uyles Black, PHI, 2nd Edition
4. *HTML and XML an Introduction*, NIIT, Prentice Hall of India Pvt. Ltd
5. *IBM PC and clones.*, Govindrajulu, B. Tata McGraw-Hill, 2012.

**18EN600**

**Technical Writing**

**2 0 0 2**

**Course Contents:**

**Unit 1**

Introduction to the Course – What is technical writing and how is it different from writing in general? Error detection – Technical Vocabulary. Mechanics of writing: Grammar rules – punctuation - spelling rules - tone and style-graphical Representation.

**Unit 2**

Different kinds of written documents: Definitions- descriptions- instructions-recommendationsmanuals - reports – proposals, Instructions manual, job applications with ResumeIntroduction to Writing dissertations, papers, and technical proposals

**Unit 3**

Technical paper writing: Library research skills- documentation style - document editing – proof reading - formatting Practice in oral communication: Group Discussion, Interviews, and Technical presentations

**References**

1. Hirsh, Herbert. L “Essential Communication Strategies for Scientists, Engineers and Technology Professionals”. II Edition. New York: IEEE press, 2002
2. Anderson, Paul. V. “Technical Communication: A Reader-Centred Approach”. V Edition. Harcourt Brace College Publication, 2003
3. Strunk, William Jr. and White. EB. “The Elements of Style” New York. Alliyen& Bacon, 1999.
4. Riordan, G. Daniel and Pauley E. Steven. “Technical Report Writing Today” VIII Edition (Indian Adaptation). New Delhi: Biztantra, 2004.

**Learning Outcome:** This course introduces the students to the elements of technical style, the basic elements of formal correspondence, technical paper writing skills and methods of documentation and help them to improve oral presentation skills in formal contexts.

**Evaluation Pattern – R.13 & R.16**

**18OEL664**

**BhagavadGita and Personality Development**

**2 0 0 2**

**Course Contents:**

**Unit 1**

NATURE AND SCOPE OF PERSONALITY : Connotation of the term Personality , Some Scientific Definitions of Personality , Determinants of Personality in Indian View , A Path fromPhysical to Spiritual Sphere

**Unit 2**

NATURE OF PURUSARTHAS: Essentials of Dharma Purusartha, Connotation of Dharma, Concept of Dharma, Sources of Dharma, the Universality of Dharma, Tree of Dharma

### Unit 3

INTRODUCTION TO BHAGAVAT GITA : Bhagavat Gita - The Nectar ,Importance of the Bhagavad Gita, The Bhagavad Gita - Its Symbolic Spirit , The Bhagavad Gita - Its Context

### Unit 4

DISCIPLINES OF PERSONALITY DEVELOPMENT IN THEBHAGAVADGITA: Lord Krsna - The Real Teacher, Arjuna - A Model Student, Knowledge of Oneself - Essential for One's Betterment, Svadharma and a State of Equanimity, Discipline of Non-attachment, Svadharma - A Kind of Yajna , Svadharma and & Meditative Discipline

### Unit 5

PERSONALITY DEVELOPMENT IN PAST & PRESENTA RETROSPECT AND PROSPECT-Retrospective Theme, Constituents of Personality Development, Western Views on Personality

#### Text book / Reference books

1. Personality development in the Bhagavad Gita - a critical study , Archak K B, 2012
2. Bhagavad Gita – translation by Swami VidyamritanandaPuri, Mata Amritanandamayi Math

## Evaluation Pattern – R.13 & R.16

18OEL665

CHEMICAL ASPECTS OF FORENSIC SCIENCE

2 0 0 2

### Course Contents:

#### Unit 1 Chemical Analysis

Origin and need for forensic science - trace and contact evidence, marks and impression, examination of documents, blood stain analysis, explosives, chemical analysis of explosives.

#### Unit 2 Analysis of Drugs

Narcotics, classification of drugs, specific drugs- Psychotropic drugs, chemical screening of drugs, chemical extraction and sample preparation, chemical identification of drugs using analytical methods.

#### Unit 3 Fingerprinting

History of fingerprinting, principles of fingerprinting, constituents of latent finger marks, fingerprint detection, chemical methods of detection

#### Unit 4 Toxicology Analysis

Introduction to Toxicology, alcohol and human body, testing of blood alcohol concentration, Toxins & Biological Poisons, Measuring Toxicity as LD50, sample and analysis, inorganic poisons, nerve agents, radioactive toxins, tests for toxins.

#### Unit 5 Postmortem

Introduction, tissue and fluid specimens, specimen collection and storage, extraction procedure, analytical techniques, interpretation, case studies

#### REFERENCE BOOKS:

1. Lawrence Kobilinsky, *Forensic Chemistry Handbook*, John Wiley & Sons, New Jersey, 2012
2. David E. Newton, *Forensic Chemistry, Facts On File, Inc, New York, 2007*
3. Jay A. Siegel, *Forensic Chemistry fundamentals and applications*, Wiley Balckwell.
4. Suzanne Bell, *Drugs, Poisons, and Chemistry, Facts On File, Inc. New York, 2009.*
5. Ashraf Mozayani, Lionel P. Raymon, *Handbook Of Drug Interactions -A Clinical And Forensic Guide, Humana Press Inc., 2004.*

## Evaluation Pattern – R.13 & R.16

**Course Contents:****Unit I Introduction**

**What Makes Knowledge Scientific:** Non-scientific methods vs. scientific methods of inquiry. **Philosophy of Science:** Epistemology and ontology, objectivist-positivist vs. constructivist-interpretivist paradigm, quantitative vs. qualitative research. **The Research Cycle:** Relationship between theory and observations, Cause and effect, Relations and roles of constructs and variables. **The Research Process-**From researchable problem to research question, From theory to hypothesis, Research approach (quantitative, qualitative or mixed-methods), Objectives, Research design (survey design or experimental design), Research methods: Collecting data, Analysing data; Interpreting results (discussion, conclusion and implications), Publishing results. **What do you look for in a good research study?:**Criteria for good research, Attributes of a good theory: Explanatory power, Falsifiability, Logical consistency, Parsimony, Empirical testability.

**Unit II Research Designs**

**Research Designs:** Experiments, Quasi-experimental designs, Cross-sectional comparative or correlational designs. **How Do You Measure Something? – Operationalisation-**Levels of measurement: Nominal (or categorical), Ordinal, Scale (or interval), Ratio; Measurement validity: Internal validity, External validity; Measurement Reliability: Stability, Equivalence; Measurement tools or instruments: Observations, Surveys, questionnaires, tests, Scales and response options. **Sampling:** Probability sampling: Simple random sampling, Systematic sampling, Cluster sampling, Stratified sampling; Non-probability sampling: Convenience sampling, Purposive sampling: quota sampling and snowball sampling.

**Unit III Analysing Quantitative Data with SPSS and Interpreting Results**

Introduction to SPSS-Entering data into SPSS. Descriptive Statistics to Summarise and Present Data-Frequencies, graphs, tables, Measures of central tendency and dispersion: Arithmetic mean, Median, Mode, Range, Variance, Standard Deviation.

**Unit IV Analytical or Inferential Statistics to Test Hypotheses**

**Analytical or Inferential Statistics to Test Hypotheses** - Normal distribution, Null hypothesis ( $H_0$ ) and alternative Hypothesis ( $H_1$ ), Type I and II Errors and the significance level. **Parametric vs. Non-Parametric Tests-**Conditions for parametric tests. **Measuring Differences Between Groups:** Chi-Square, t-Test, Univariate ANOVA, Multivariate ANOVA. **Exploring Relationships Between Variables:** Cross Tabulations, Correlation, Linear Regression

**Unit V Publishing Results**

**Publishing Results-**Writing for professional research journals, Major components of a research paper, Process of publishing a journal article. **Ethical Considerations** - Informed consent, Confidentiality, Do no harm, Research integrity.

**Reading Material:**

1. Bhattacharjee, A. (2012). Social science research: Principles, Methods, and Practices. Textbooks Collection. Book 3. Retrieved from [[http://scholarcommons.usf.edu/cgi/viewcontent.cgi?article=1002&context=oa\\_textbooks](http://scholarcommons.usf.edu/cgi/viewcontent.cgi?article=1002&context=oa_textbooks)].
2. Kothari, C.R. (2004). Research Methodology. Methods and Techniques (2nd revised edition). New Delhi, India: New Age International Publishers. Retrieved from [<http://www.modares.ac.ir/uploads/Agr.Oth.Lib.17.pdf>].
3. Kumar, R. (2011). Research Methodology. A step-by-step guide for beginners (3rd edition). Los Angeles, CA: Sage. Retrieved from [<http://www.sociology.kpi.ua/wp->

## Evaluation Pattern – R.13 & R.16

18OEL667

Research methods for Social Sciences – II

2002

### Course Contents:

#### Unit I: Historical, Philosophical, Ethical Context:

Scientific vs. non-scientific approaches to learning: Stammtisch psychology, Ontological and epistemological approaches to learning- Hermeneutics, Phenomenology, Pragmatism-Comparisons with quantitative approaches: strengths & weaknesses of both approaches, Ethical considerations and mandates in Social Sciences Research.

#### Unit II: Aspects and Characteristics of Qualitative Research

Theoretical and conceptual issues, How the choices of methodology are linked to broader theoretical and conceptual issues: consider the appropriateness of different methodologies and types of evidence chosen for specific research questions. Evaluating published studies in social science fields: Examining the logic of presented arguments, their related chosen methodologies, and the relationship between the evidence presented and the argument. Understanding the power and purpose of the Literature Review in Qualitative Research: Defining the primary Research Question of interest. Lab Component: Identify interest area for small group research study

#### Unit III: Qualitative Research Methods

Required data collection skills for the researcher: Observations, Listening Skills, mapping skills, communication, flexibility, Importance of self-reflection/observation/awareness. Lab Component: Application of skills learned through practical exercises.

Design of Study: Methods of Data Collection-Interview; Survey; Focus Group; Document Analysis; Survey, Participant Observation, Case Studies, Media Materials (audio, video, photo, etc.) Written sources (documents, biographies, diaries); Documentary/primary sources. Lab Component: Differences between survey and interview questions. Conducting the Focus Group: class project.

Understanding Focus Group design for Qualitative data: Lab Component: data collection for small group study.

#### Unit IV: Data analysis methods

Overview of conventional & more contemporary methods: Content Analysis, Comparative Analysis, Thematic Analysis, Framework Analysis. Integrative Analysis: Strengthening reliability of results and minimizing researcher bias. Lab Component: Analysis of collected data in small groups using Integrative approach.

#### Unit V: Interpretations, findings, synthesis of project into scientific paper

After the initial Code Structure and coding of data: The role of interpretation in research results,



Presentation of results in systematic, scientific manner. Overview of steps in writing scientific research paper: Strengthening each section of paper, Comprehensive, systematic reporting of methodology utilized, Proper citations, and citation reporting within text and References sections of paper.

## Readings:

1. Maggi Savin-Baden and Claire Howell Major (2010). *New Approaches to Qualitative Research Wisdom and Uncertainty*.
2. Robert K. Yin (2011). *Qualitative Research from Start to Finish*.
3. Yvonne Darlington and Dorothy Scott (2002). *Qualitative research in practice -Stories from the field*.

**Learning Outcome:** This course involves lecture, group discussion, and a practical hands-on lab component for each of the Units. The course will help prepare students to develop confidence and competence in designing qualitative research, executing the study, analyzing the data, and presenting findings in an academic paper. Students are expected to complete required readings for participation in class discussions. This course provides training for the graduate students planning to conduct qualitative research in a variety of different settings.

## Evaluation Pattern – R.13 & R.16

18OEL668

Qualitative Research Methods: Content Analysis

2002

When people talk with others about any topic and go about their daily lives, what they say and do are a continuous stream. So as to make sense of this, we all parse the continuous stream into parts, even if we are not aware that that's what we do.

In contrast, researchers parse what people do and say in a reflective and conscious way. That parsing is informed by a prism through which researchers describe the world they are describing. The prism is the theory (are the theories) they hold.

When some cognitive psychologists do this, they categorize people's behaviors. They also believe that there is a psychological entity (say, a mental model) that leads to the behaviors they observe. These behaviors are observable. The psychological entity that organizes and leads to these behaviors is invisible, not available to observation. Their traces are the behaviors we can observe.

An assumption psychologists have is that the psychological entity gives rise to behaviors and when we observe these behaviors, we can infer the psychological entity that produces them. Psychological entities are the black box that psychologists attempt to describe.

The course is founded on these ideas. We will listen to what people say about aspects of their lives that interest you and them, and we will then analyze what they say in an attempt to determine the categories that are part of the black box we want to describe.

We will also attempt to place these psychological entities in a cultural framework which will add richness and subtlety to the psychological entity.

If we can successfully make this description, we can then know what places could be addressed in intervention programs, such as women empowerment programs, and how these programs could be informed by the culture in which women are a part.

## Course Organization

The course will be 2 weeks long, with 3 meetings per week and with each class lasting 4 hours. The total number of class hours will be 24.

- Meeting 1: General presentation of the course.  
Exercises on content analysis  
Between meeting 1 and 2 the students will interview others about a topic of interest.
- Meeting 2: Building categories based on content analysis of interviews  
Deciding on a topic of research for each group
- Meeting 3: Each group will build an interview in class.  
Between meeting 3 and 4, each group interviews people.
- Meeting 4: Each group presents its data from interviews and preliminary categories  
Between meeting 4 and 5, each group creates what it believes is the mental models of people they interviewed.
- Meeting 5: Each group presents its work to the entire class. First “draft”.  
Between meeting 5 and meeting 6, each group refines its presentation.
- Meeting 6: Each group presents its work to the entire class. Final draft.  
Course summary and discussion of implications for the development of intervention programs

## Course requirements

- Attending each class
- Completing all assignments

## Grades

- PhD students:
  1. Presentation of their work in meeting 6.
  2. Writing a paper describing research conducted using content analysis as the basis for the paper.
- MSW students:
  1. Presentation of their group work in meeting 6.

## Bibliography

1. Strauss, S., & Shilony, T. (1994). Teachers' models of children's minds and learning. In L. Hirschfeld & S. Gelman (Eds.), *Mapping the mind: Domain-specificity in cognition and culture* (pp. 455-473). Cambridge, UK: Cambridge University Press. doi: 10.1017/CBO9780511752902.019  
<https://www.researchgate.net/search/Search.html?type=publication&query=strauss%20and%20shilony>
2. Charmaz, K. (1996). The search for meaning: Grounded theory. In J. A. Smith, R. Harre & L. Van Langenhove (Eds.), *Rethinking methods in psychology* (pp. 27-49). London: Sage Publications.  
[http://www.sxf.uevora.pt/wp-content/uploads/2013/03/Charmaz\\_1996.pdf](http://www.sxf.uevora.pt/wp-content/uploads/2013/03/Charmaz_1996.pdf)
3. Corbin, J., Strauss, A. (1990). Grounded theory research: Procedures, canons and evaluative criteria. *Zeitschrift fur Soziologie*, 19, 418-427. <http://www.zfs-online.org/index.php/zfs/article/viewFile/2741/2278>

## Evaluation Pattern – R.13 & R.16

18OEL669

Introduction to Vulnerability Mapping and Analysis

2 0 0 2

## Course Contents:

**Unit I:** Introduction to Vulnerability Studies

Introducing Vulnerability - An introduction to vulnerability covering main definitions and concepts such as: exposure, risk, hazards, adaptation, coping, and resilience.

## **Unit II: Multidimensional Nature of Vulnerability**

Exploring vulnerability from a multidimensional approach: including multi-stressor vulnerabilities, social, environmental, institutional, economic, and biological dimensions. Vulnerability Mapping and Intervention Design, Vulnerability Mapping for Sustainable Development

## **Unit III: Mapping of vulnerabilities and Indicators**

Mapping Vulnerability - An overview of the practice of mapping vulnerability, looking into the evolution of vulnerability mapping practices and theory. Vulnerability Mapping Frameworks - An exploration of the various primary vulnerability mapping frameworks and theoretical models, including MOVE, BBC, PAR, etc.

## **Unit IV: Hazards and Indicators**

Breaking down the components of vulnerability: an in-depth look into the nature of hazards and indicators, and their inherently contextual requirements.

## **Unit V: Methods and Tools for Vulnerability Assessment**

Methods and Tools for Vulnerability Assessment - An overview of the existing VM assessment toolkits and the methods contained therein. Methodologies for data collection and analysis - Covering traditional and innovative methods of data collection and analysis, including GIS, qualitative methods, etc. Practical Assignment - A comprehensive assignment that will draw upon the preceding units to apply the methods and theories pertaining to vulnerability mapping.

## **References:**

1. Proposed Updated Terminology on Disaster Risk Reduction: A Technical Review UNISDR
2. Vulnerability as Concept, Model, Metric, and Tool, Benjamin Wisner.
3. Cardona, Omar D. "The need for rethinking the concepts of vulnerability and risk from a holistic perspective: a necessary review and criticism for effective risk management." *Mapping vulnerability*. Routledge, 2013. 56-70.
4. Turner, Billie L., et al. "A framework for vulnerability analysis in sustainability science." *Proceedings of the national academy of sciences* 100.14 (2003): 8074-8079.
5. Birkmann, Joern, et al. "Framing vulnerability, risk and societal responses: the MOVE framework." *Natural hazards* 67.2 (2013): 193-211.
6. Birkmann, Joern. "Risk and vulnerability indicators at different scales: Applicability, usefulness and policy implications." *Environmental hazards* 7.1 (2007): 20-31.
7. Moret, Whitney. "Vulnerability assessment methodologies: A review of the literature." *Washington, DC: FHI* 360 (2014).
8. Ulrichs, Martina, et al. "Climate Change & Food Security Vulnerability Assessment. Toolkit for assessing community-level potential for adaptation to climate change." (2015).

## **Evaluation Pattern – R.13 & R.16**