

BHARATHIAR UNIVERSITY, COIMBATORE.
M. Sc. CHEMISTRY DEGREE COURSE (AFFILIATED COLLEGES)
(Effective from the academic Year 2016 - 2017 onwards)

SCHEME OF EXAMINATIONS

Study Components	Course Title	Inshrs/ Week	Exam				Credits
			Dur. Hrs.	CIA*	Univ Exam	Total	
Semester I							
Paper I	Organic Chemistry – I (Organic Reaction Mechanism)	5	3	25	75	100	4
Paper – II	Inorganic Chemistry – I (Inorganic Rings and Nuclear chemistry)	5	3	25	75	100	4
Paper – III	Physical Chemistry I (Group theory nanoscience and Computers in Chemistry)	5	3	25	75	100	4
Practical - I	Organic Chemistry – I	4	--	--	--	--	--
Practical – II	Inorganic Chemistry – I	4	--	--	--	--	--
Practical – III	Physical Chemistry - I	4	--	--	--	--	--
Elective – I		3	3	25	75	100	4
Semester II							
Paper – IV	Organic Chemistry – II (Molecular rearrangements and Photochemistry)	5	3	25	75	100	4
Paper _ V	Physical Chemistry II (Quantum chemistry and nanomaterials)	5	3	25	75	100	4
Paper – VI	Physical methods in Chemistry I	5	3	25	75	100	4
Practical - I	Organic Chemistry – I	4	6	40	60	100	4
Practical – II	Inorganic Chemistry – I	4	6	40	60	100	4
Practical – III	Physical Chemistry - I	4	6	40	60	100	4
Elective – II		3	3	25	75	100	4
Semester III							
Paper -VII	Organic Chemistry - III(Chemistry of natural Products)	5	3	25	75	100	4
Paper – VIII	Physical Chemistry – III (Thermodynamics)	5	3	25	75	100	4
Paper –IX	Physical Methods in Chemistry II	5	3	25	75	100	4
Practical - IV	Organic Chemistry – II	4	--	--	--	--	--
Practical – V	Inorganic Chemistry – II	4	--	--	--	--	--
Practical – VI	Physical Chemistry – II	4	--	--	--	--	--
Elective – III		3	3	25	75	100	4
Semester IV							
Paper – X	Inorganic Chemistry – II (Coordination Chemistry)	5	3	25	75	100	4

Paper IX Physical Chemistry IV (Reaction Kinetics and Electrochemistry)	5	3	25	75	100	4
Paper – XII Polymer Technology	5	3	25	75	100	4
Practical - IV Organic Chemistry – II	4	6	40	60	100	4
Practical – V Inorganic Chemistry – II	4	6	40	60	100	4
Practical – VI Physical Chemistry – II	4	6	40	60	100	4
Elective – IV (Option given to choose either project work or Elective paper)	3	3	-	-	100**	4
Practical Viva	--		50		50	2
Total					2250	90

Electives: List of group elective papers (colleges can choose any one of the group papers as electives)

	Group A	Group B	Group C
Paper I/Sem I	Dye Chemistry	Green Chemistry	Green Chemistry
Paper II/ Sem II	Water Pollution and Industrial Effluents treatment	Water Pollution and Industrial Effluents treatment	Advanced Polymeric materials
Paper III/ Sem III	Organic Synthetic Methodology, Oxidation and Reduction	Medicinal Chemistry	Kinetics of polymerization
Paper IV/ Sem IV Theory paper (or) Project work	Industrial Chemistry	Applied Electro Chemistry	Pharmaceutical Chemistry

* Includes 25 & 40% continuous internal assessment marks for theory and practical papers, respectively.

** For Project report - 80%; Viva-voce - 20%

Note :

The syllabus for the above papers (except **Paper –II -INORGANIC CHEMISTRY – I** (Inorganic Rings and Nuclear chemistry) **PAPER III- Physical chemistry – I (Group Theory, Nanoscience and Computers in Chemistry and** Paper – X **INORGANIC CHEMISTRY – II** (Coordination Chemistry) be the same as prescribed for the academic year 2015-16. The revised Syllabus for the above papers **are furnished below:**

Semester I: Subject title : **Paper –II -INORGANIC CHEMISTRY – I** (Inorganic Rings and Nuclear chemistry)
No.of hours: 75 hrs

Subject Description :

This paper presents an idea about inorganic ring systems and clusters and Nuclear Chemistry

Goals :

To enable the students to learn some principles and theories in inorganic and solid state chemistry and nuclear chemistry

Objectives :

On successful completion of the course the students should have an exposure to Inorganic clusters and nuclear chemistry

Contents

UNIT – I

Heterocatenation- Silicate minerals-classification-Ortho,Pyro, Cyclic, Chain, Sheet, Three dimensional silicates- Zeolites-Isopoly and Heteropoly anions-Cages-boranes- Carboranes- Clusters – Metal clusters-Classification-Carbonyl clusters–Low Nuclearity carbonyl clusters(Dinuclear, trinuclear and tetra nuclear carbonyl clusters)-High Nuclearity carbonyl clusters-Wades rule-Halide type clusters ($[\text{Re}_2\text{X}_8]^{2-}$, $[\text{Re}_3\text{X}_9]$, $[\text{W}_4(\text{OR})_{12}]$, $[\text{Mo}_6\text{Cl}_8]^{4+}$, $[\text{Nb}_6\text{Cl}_{12}]^{2+}$ - Cheveral phases and naked clusters-Organometallic clusters

UNIT – II

Borazines – phosphonitrilic compounds – sulphur - nitrogen ring compounds.

Metallic state – free electron and band theories – non stoichiometry – point defects in solids – Schottky - Frenkel defects – linear and dislocation effects.

UNIT – III

Electrical properties of solids: Conductors and nonconductors Conductivity in pure metals and alloys– superconductors –Occurrence of superconductivity- BCS theory-Type-I and Type-II, and High temperature (HT) superconductors- Preparation of HT superconductors-critical temperature – persistent currents- Meissner effect.

Magnetic properties-Diamagnetism, Paramagnetism and Ferromagnetism- Langevin equation-- Curie's law-Zener's theory-Domain Structure.

Thermoelectric properties – Phenomenon thermoelectricity- Seeback, Peltier and Thomson effects – Synthesis of Thermoelectric materials- Applications of thermoelectric materials.

UNIT – IV

Nuclear chemistry-the nuclues-subatomic particles and their properties –Stability of nucleus-binding energy- N/P ratio, packing fraction-nuclear forces-Meson theory-Nuclear models-Liquid drop model-shell model-mode of radioactive decay- α , β , γ decay-Half life period-nuclear isomerism-internal conversion.

UNIT – V

Nuclear reactions (Capture, Particle-particle, spallation, photodisintegration)- Q-value, coulombic barrier, cross section. Fission, fusion & theories of fission- Pinch Effect-Atom bomb, Hydrogen and Plutonium bomb-Fissile and fertile isotopes – U^{233} , U^{235} , Pu^{239} , Th^{232} , Radioactive series (U, Th, Ac and Np series)- Atomic power projects in India, stellar energy-Application of radio isotopes-hot atom chemistry.

References :

1. Cotton and Wilkinson : Advanced inorganic Chemistry, Wiley Eastern (P), Ltd., 1968
2. Gurdeep and Harish : Advanced inorganic Chemistry, Geol Publishing House
3. G.M.Arora : Solid State Chemistry
4. R.A.Alberty and Silbey : Solid State Chemistry
5. J.P.Srivastava : Elements of Solid State Physics
6. S. Glasstone, Source book of atomic Energy, Van Nonstrand Co., 1969.
7. H.J. Arniker, Essentials of nuclear chemistry, 2nd edition Wiley eastern Co.,1987.

Semester I:PAPER III- Physical chemistry – I (Group Theory, Nanoscience and Computers in Chemistry)

No.of hours: 75 hrs

Subject Description:

This paper presents an idea about group theory and the basic concepts of nanoscience and the computer applications in Chemistry.

Goals :

To enable the students to learn group theory, nanoscience and computer application concept

Objectives :

On successful completion of the course the students should have an exposure to the group theory and nano technology and a basic idea of computers in chemistry.

UNIT - I

Symmetry elements and symmetry operations: definition of identical and equivalent elements configurations- symmetry operations and symmetry elements-rotation-axis of symmetry- reflections symmetry planes-inversion center-improper rotations-rotation-reflection axis-effect of performing successive operations (commutative and non - commutative) - inverse operations.

Groups and their basic Properties: Definition of a group -basic properties of a group-definition of Abelian group-isomorphic group-similarity transformation and classes-group multiplication tables-symmetry classification of molecules into point groups (Schoenflies symbol only) difference between point group and space group.

UNIT-II

Definition of reducible and irreducible representations-irreducible representations as orthogonal vectors-direct product rule-the great orthogonality theorem and its consequences (statement only proof not needed)-determinations of the characters for irreducible representation of C_{2v} and C_{3v} point groups using the orthogonality theorem. Calculation of character values of reducible representations per unshifted atom for each type of symmetry operation (Character table may be provided to the students)-determination of total Cartesian representation—determination of direct sum from total Cartesian representation.

Group theory and vibrational spectroscopy-vibrational modes as basis for group representation symmetry selection rules for IR and Raman spectra (mutual exclusion principle)-classification of vibrational modes.

Application of group theory to chemical bonding

- Hybridization schemes for σ bonding in AB_4 (T_d) type (methane).
- Hybridization schemes for π bonding in AB_3 (D_{3h}) type (boron trichloride).

UNIT III

Nanoscience

Definition of nanodimensional materials - Historical milestones - Properties at the nanoscale dimension- Physical basis and principles. 0D, 1D, 2D, 3D Structures. Graphite to buckyballs to Carbon nanotubes (CNT). Single and Multiwalled CNT. Synthesis of – Nanotubes (Laser ablation, Electric Arc method, Catalytic Chemical Vapour Deposition-Homogeneous and heterogeneous including mechanism of growth -tip based root based), Functionalisation of nanotubes,

UNIT IV

Nanowires and nanorods (Template assisted synthesis- Pressure, Electrochemical, PVD, CVD and MOCVD methods, Template filling - Melt and solution filling, Electrospinning).

Nanofabrication: Top-down approach – Nanolithography - Photo, Deep ultraviolet, X-ray, Electron beam, and Ion beam lithography. Soft lithography - dip pen nanolithography. Bottom-up approach - STM/AFM atomic manipulation. Chemical method(Sol-gel synthesis).

UNIT-V

Introduction to computers and computation in chemistry

Basic structure and functioning of computers with PC as an illustrative example- memory. I/O devices secondary storage-computer languages-operating systems with DOS as an example-introduction to UNIX and WINDOWS-data processing, principle of programming- algorithms and flow charts. Data entry devices for sequential processing-data entry devices for direct access processing-data communication concepts: LAN, WAN, e-mail internet concept; computer virus; soft ware packages.

REFERENCES:

1. F.A.Cotton : Chemical applications of Group theory
- 2 M. Orchin and H.H. Jaffe : Symmetry, Orbital and spectra
3. G. Davidson : Introductory Group theory for Chemists
- 4 K.V. Raman : Computers in Chemistry
5. E. Balagurusamy and Deenadialu : Introduction to Computer
6. E. Balagurusamy : Programming in C
7. Jackie Ying - Nanostructured Materials, Academic Press; 1st edition, 2001.
8. Gregory L. Timp – Nanotechnology, American Institute of Physics; 1st edition, 1998.
9. Guozhong Cao – Nano structures and nano materials: Synthesis, properties and Applications- Imperial College Press (2004)
10. K. Eric Drexler- Engines of Creation. Anchor Books/Doubleday
11. K. Eric Drexler- Nanosystems: Molecular Machinery, Manufacturing, and Computation. John Wiley & Sons, Inc.: New York, 2001.
12. Robert A. Freitas Jr.- Kinematic Self-Replicating Machines. Landes Bioscience: Georgetown, TX. 2004
13. J. Storrs Hall, Nanofuture: What's Next For Nanotechnology, Prometheus Books, 2005.
14. NorioTaniguchi- Nanotechnology - Oxford University Press, 2005.

Semester IV: Paper – X- **INORGANIC CHEMISTRY – II** (Coordination Chemistry)

No.of hours: 75 hrs

Subject Description :

This paper presents basic principles of coordination chemistry and bioinorganic chemistry .

Goals :

To enable the students to learn some principles and theories in coordination, organometallic chemistry and bioinorganic chemistry .

Objectives :

On successful completion of the course the students should learn basic principles, important theories and applications of coordination chemistry.

Contents

UNIT – I

Crystal field theory – spectrochemical series – molecular orbital theory –comparison of MOT and CFT- π - bonding – magnetic behaviour of the transition metal ions (Paramagnetic and diamagnetic properties, cooperative magnetism). Thermochemical correlation.

UNIT – II

Term symbols for the 3d-block elements and their ions – Orgel diagram (d^3 and d^5 only) –Tanabe-Sugano diagram for Co^{3+} system – John-Tellar distortions – spin-orbit coupling –Nephelauxetic effect – charge transfer spectra.-Racah parameters. Substitution reactions in square planar and octahedral complexes – trans effect – redox reactions (Inner and Outer sphere mechanism)

UNIT – III

d-Block metal carbonyls – General preparation, properties structure and Spectroscopic properties (^{13}C and IR) EAN Rule–Preparation, properties and structure of Iron carbonyls – Preparation and Structure of $Fe_2(CO)_9$ and $Co_4(CO)_{12}$ – Carbonyl hydrides $[HMn(CO)_5]$, $[HCo(CO)_4]$, $[H_2Fe(CO)_4]$ (Preparation and chemical reaction only)- Complexes of molecular nitrogen and oxygen (synthesis and reactions). Isolobal analogies.

UNIT – IV

Cyclopentadienyl complex-Ferrocene – synthesis, structure and reactions (Acetylation, aminomethylation, metalation, Nitration and Halogenation). Homogeneous catalysis by coordination compounds – hydroformylation using $Co(CO)_4H$ – Carboxylation of methanol – hydrogenation of alkenes (Wilkinson's catalyst)-Wacker oxidation of alkenes-Alkene metathesis (Grubb's catalyst)-Reppé synthesis(Nickel based catalyst) -Vaska's compound – Zeise salt.

UNIT – V

The Inorganic composition of cells- Sodium and potassium transport- Cytochromes (electron transfer)-Zinc enzymes(carbonic anhydrase) – Peroxidases-Oxidases-Oxygenases-Photosynthetic oxygen production-Nitrogen fixation (*in vivo* and *in vitro*). Hemoglobin – myoglobin - cyanocobalamin – chlorophyll (structure and functions). Chelation therapy, antitumour agents - *cis*-platin.

References

1. Shriver and Atkins, Inorganic Chemistry, Fifth Edition.
2. K.F. Purcell and J.C.Cotz, Inorganic chemistry, , Fifth Edition.
3. James E. Huheey, Ellen A. Keiter and Richard L.Keiter : Inorganic Chemistry, IV Edn., 1993
4. Cotton and Wilkinson : Advanced inorganic Chemistry, Wiley Eastern (P), Ltd., 1968
5. H.J.Emeleus and A.G.Sharp : Modern aspects of Inorganic Chemistry, IV Edn., 1989
6. R.S.Drago : Physical methods in Inorganic Chemistry, 1978
7. R.C.Mehrotra and A.Singh : Organometallic Chemistry