CHEMICAL SCIENCES

Programme Code: CHEM00

Programme Outcome:

- Firm foundation in the fundamentals and application of current chemical and scientific theories including those in Analytical, Inorganic, Nuclear and Physical Chemistry.
- Ability to design and carry out scientific experiments as well as accurately record and analyse the results of such experiments.
- Skill development in problem solving, critical thinking and analytical reasoning as applied to scientific problems.
- Ability to clearly communicate the results of scientific work in oral, written and electronic formats to both scientists and the public at large.
- Appreciate the central role of chemistry in DAE programmes and use this as a basis for ethical behaviour in issues facing chemists including an understanding of safe handling of chemicals, environmental issues and key issues facing our society in energy, health and medicine.

DETAILED COURSE COURSES

Foundation Courses					
Sr. No	**Subject Title**	**Course Code**	**Hours**		**Credits**
			L	**P**	
1	Mathematics, Quantum Chemistry & Computational	CY501	40	10	3
2	Analytical Chemistry	CY502	42	6	3
3	Material Science	CY503	28	4	2
4	Radiation Detection and Measurements	CY504	30	0	2
5	Nuclear and Radiochemistry	CY505	42	6	3
6	Thermodynamics	CY506	15	0	1
	FOUNDATION TOTAL		197	26	14

Core Courses					
Sr. No	**Subject Title**	**Course Code**	**Hours**		**Credits**
			L	**P**	
1	Lasers	CY601	14	2	1
2	Electronics & Chemical Instrumentation	CY602	27	6	2
3	Production and Applications of Radioisotopes	CY603	30		2
4	Reactor Physics and Reactor Chemistry	CY604	15		1
5	Molecular Structure & Spectroscopy	CY605	28	4	2
6	Radiation and Photochemistry	CY606	28	4	2
7	Chemistry in Nuclear Fuel Cycles	CY607	45		3
8	Advanced Chemical Kinetics & Dynamics	CY608	13	4	1
9	Health Physics and Radiation Biology	CY609	15	0	1
10	Safety in Chemical and Radiochemical labs	CY 611	15		1
	CORE TOTAL		230	20	16

ELECTIVE COURSES

Elective Courses				
Sr. No	**Subject Title**	**Course Code**	**Hours (L)**	**Credits**
1	Nanomaterials, Chemical Sensors	CY701	15	1
2	Soft Condensed Matters	CY702	15	1
3	Nuclear Probes for Material Characterization	CY703	15	1
4	Molecular Bio organics	CY704	15	1
5	Laser Spectroscopy	CY705	15	1
6	Actinide Chemistry	CY706	15	1
7	Computational Chemistry	CY707	15	1
8	Advanced NMR Spectroscopy	CY708	15	1
9	Atmospheric Chemistry	CY709	15	1
10	Statistical Analysis	CY710	15	1
	ELECTIVES TOTAL		45	3

Non-Subject Assignments			
Sr. No	**Subject Title**	**Course Code**	**Credits**
1	Viva Voce	CY591	4
2	Mini Project (300 hrs, 6 W half day, 4 W Full day)	CY592	9
3	Seminar	CY593	4
		TOTAL	**17**

L: Theory Hr., P: Lab Hr., 1 Credit = 15 Theory Hrs. / 30 Lab. Hrs

CORE COURSES COORDINATOR

Chief Coordinators: Dr. Dimple Dutta (HRDD, Extn.: 22308, E-Mail: dimpled@barc.gov.in)
Chief Coordinators: Dr. Sumit Kumar (RACD, Extn: 20644 / 25958, E-Mail: sumitk@barc.gov.in)

Foundation & Core Courses		
Course	**Coordinators**	**Email ID**
Mathematics, Quantum Chemistry & Computational Methods (CY501))	Dr. A. K. Pathak (ChD)	akpathak@barc.gov.in
Analytical Chemistry (CY502))	Dr. Remya Devi P.S. (ACD)	psremya@barc.gov.in
Material Science (CY503)	Dr. Seemita Banerjee (RPCD)	seemita@barc.gov.in
Radiation Detection & Measurement (CY504)	Dr. Dhanadeep Dutta (RCD)	deep@barc.gov.in
Nuclear & Radiochemistry (CY505)	Dr. Chhavi Agarwal (RCD)	cagarwal@barc.gov.in
Thermo-dynamics (CY506)	Dr. R.A. Jat (PDD)	avtar@barc.gov.in
Lasers (CY601)	Dr. A. K. Singh (HRDD)	aksingh@barc.gov.in
Electronics & Chemical Instrumentation (CY602)	Shri R. Manimaran (ChD)	rmani@barc.gov.in
Production & Applications of Radioisotopes (CY603)	Dr. Drishty Satpati (RPhD)	drishtys@barc.gov.in
Reactor Physics & Reactor Chemistry (CY604)	Dr. V.S. Tripathi (RPCD)	vst_apcd@barc.gov.in
Molecular Structure & Spectroscopy (CY605)	Dr. Dimple Dutta (HRDD)	dimpled@barc.gov.in
Radiation & Photochemistry (CY606)	Dr. A. Barik (RPCD)	atanu@barc.gov.in
Chemistry in Nuclear Fuel Cycle (CY607)	Dr. Pranaw Kumar (FCD)	pranaw@barc.gov.in
Chemical Kinetics and Dynamics (CY608)	Dr. P. Mathi (RPCD)	mathip@barc.gov.in
Health Physics and Radiobiology (CY609)	Dr. B.N. Pandey (RB & HSD)	bnp@barc.gov.in
Safety in Chemical and Radiochemical (CY611)	Dr. Jaison P.G. (FCD)	jaipg@barc.gov.in

ELECTIVE COURSES COORDINATOR

Elective Courses		
Course	**Coordinators**	**Email ID**
Nanomaterials, Chemical Sensors (CY701)	Dr. B.P. Mandal (ChD)	bpmandal@barc.gov.in
Soft Condensed Matters (CY702)		
Nuclear Probes for Material Characterization (CY703)	Dr. S.K. Sharma (RCD)	skumars@barc.gov.in
Molecular Bio organics (CY704)	Dr. Dibakar Goswami (BOD)	dibakarg@barc.gov.in
Laser Spectroscopy (CY705)	Dr. J.A. Mondal (RPCD)	mondal@barc.gov.in
Actinide Chemistry (CY706)	Dr. Sumit Kumar (RACD)	sumitk@barc.gov.in
Computational Chemistry (CY707)	Dr. C. Majumder (ChD)	chimaju@barc.gov.in
Advanced NMR Spectroscopy (CY708)	Dr. Sandeep Dey (ChD)	dsandip@barc.gov.in
Atmospheric Chemistry (CY709)	Dr. P. Mathi (RPCD)	mathip@barc.gov.in
Statistical Analysis (CY710)	Dr. K.K. Swain (ACD)	kallola@barc.gov.in

FOUNDATION COURSES

CY501: Mathematics, Quantum Chemistry & Computational Methods (40 L + 10 P)

Coordinators: Dr. A. K. Pathak (ChD)
akpathak@barc.gov.in

Course Details:

- **Differential Equations & Integral Transforms**

  Introduction to differential equations: order and degree; Different methods of solution; Overview of Legendre, Lagurre and Hermite differential equations; Introduction to Fourier series, Fourier transform and Laplace transform.

- **Vector Calculus**

  Vector differentiation and integration: Concepts of gradient, divergence and curl; Laplacian operator.

- **Matrix Algebra**

  Elementary operations and elementary matrices. Solution of linear equations; Similarity transformations; Eigenvalues and eigenvectors; Diagonalization and inversion of matrices.

- **Group Theory and Symmetry in Chemistry**

  Concepts of groups, sub groups and classes; Symmetry elements, and symmetry operations; Point groups and matrix representations; Great orthogonality theorem and its importance in chemistry, Reducible and irreducible representations; Character Tables and their applications to spectroscopy, molecular geometry and chemical reactions.

- **Quantum Chemistry**

  Postulates of quantum mechanics, Classes of operator: Linear and Hermitian, Physical significance of eigen value in quantum mechanics; Boundary value problem in quantum mechanics; Exactly solvable problems: Particle in a box and ring; simple harmonic oscillator; rigid rotor and hydrogen atom; Approximation methods: Variation method; perturbation theory for time-independent and time dependent systems; Many-electron systems: Hartree- Fock theory and beyond; Chemical binding in simple molecular systems: Valence bond and molecular orbital theories; Concept of LCAO and introduction to ab-initio and semi-empirical molecular orbital calculations of molecules; Extended systems: From bonds to bands; Applications to few simple molecules.

- **Computer Programing and Numerical Methods**

  Computers and modeling in chemistry; Basics of computer programming: Variables, constants, input/output and control statements, arrays, functions, and subroutines. Computer oriented numerical methods: Newton- Raphson method for finding roots, differentiation, integrations by quadrature techniques, solutions of differential equations, diagonalization and inversion of matrices. Curve fitting. Basics of computer simulation: Monte Carlo and molecular dynamics simulations.

Course Outcomes:

- Provides the knowledge of basic and applied mathematics, quantum mechanics and computer programming for solving real problems using advanced mathematical techniques.
- Applications of group theory to understand the structure and spectroscopic results.

References

[1] M.R. Spiegel. Advanced Mathematics for Engineers and Scientists, Schaum's Outline Series (1983).
[2] K.F. Riley, M.P. Hobson and S.J. Bence. Mathematical Methods for Physics Engineering, Cambridge University Press (1998).
[3] M.R. Spiegel. Theory and Problems of Vector Analysis, Schaum's Outline Series (1981).
[4] F.A. Cotton. Chemical Applications of Group Theory, Wiley (1971).
[5] S.F.A. Kettle. Symmetry and Structure: Readable Group theory for Chemists, John Wiley (1995).
[6] A. K. Mukherjee and B. C. Ghosh. Group Theory and Chemistry: Bonding and Molecular Spectroscopy, University Press, 2017.
[7] I.N. Levine. Quantum Chemistry, Prentice-Hall (1994).
[8] A.K. Chandra. Introductory Quantum Chemistry, Tata McGraw Hill (1979).
[9] V. RajaRaman. Computer Oriented Numerical Analysis, Prentice Halls India, 3rd ed. (1999)
[10] William E. Mayo. Programming with Fortran 77, Schaum Outlines Series, McGraw Hill, International ed. (1995)

CY502: Analytical Chemistry (42 L + 6 P)

Coordinators: Dr. Remya Devi P.S. (ACD)
psremya@barc.gov.in

Course Details:

- **Introduction**

  Relevance of Analytical Chemistry in Atomic Energy Programme, Terminologies in Analytical Chemistry, Quality Assurance in Analytical Chemistry, Accreditation and its importance.

- **Separation Technique**

  Solvent extraction: Principles and Applications, Conventional solvent extraction, Liquid membranes, Bulk membranes, Supported and Emulsified liquid membrane, Super critical fluid extraction (SFE).

  Ion Exchange: Principles and Applications, Conventional ion exchange, Solid Phase Extraction (SPE) Chromatography: Principles and Applications, Gas chromatography (GC), High Performance Liquid Chromatography (HPLC), Ion chromatography (IC), Supercritical fluid Chromatography (SFC), Capillary electrophoresis.

- **Electrochemical Techniques**

  Introduction to the oxidation and reduction process, equilibrium electrochemistry, Activity, Nernst equation, Butler-Volmer equation, Tafel treatment. Potentiometry/potentiometric titration and ion Selective Electrodes (ISE), Modified electrodes.

  Electrochemical double layer, Mass transfer processes, Fick's law of diffusion, Polarisation, Voltammetry & Polarography, working electrode, reference electrode and counter electrodes,

  Votammetric techniques like; Linear sweep voltammetry, Cyclic voltammetry, Pulse and Stripping Voltammetry, Coulometry and Amperometry, Hydrodynamic voltammetry.

  Electrochemical Impedance spectroscopy and modelling of the electrochemical interface. Electrochemistry at ultramicro electrode, Scanning Electrochemical Microscopy, electrochemistry at confined geometry and detection at single molecule level, Hyphenated in-situ Spectro-electrochemical techniques.

- **Spectrochemical Techniques**

  An introduction to spectrometric methods, Performance Characteristics of instruments, Calibration of instrumental methods, Quantitative aspects of spectrochemical measurements.

  Atomic Absorption spectrometry (AAS), Sources of radiation (Hollow Cathode lamp, Continuum Source), Atom cell, Flame Atomic Absorption Spectrometry (FAAS), Electrothermal Atomic Absorption Spectrometry (ETAAS), Cold vapor Atomic Absorption Spectrometry (CVAAS), Hydride generation Atomic Absorption Spectrometry (HGAAS), Types of Interferences in AAS and Background correction methods.

  Optical Emission Spectrometry, Emission sources: Flame, Inductively Coupled plasma, Glow Discharge, DC- Arc, Inductively Coupled Plasma Optical Emission Spectrometry (ICP-OES), Types of interference in ICP-

  OES and background correction methods, Laser Induced Fluorescence (LIF).

- **Mass Spectrometry**

  Basic principle, Ion sources: Thermal Ionisation (TI), Electron Impact(EI), Inductively Coupled Plasma(ICP), Glow Discharge(GD), Laser Ablation (LA), Secondary Ionisation (SI), Resonance Ionisation (RI), Matrix Assisted Laser Desorption and Ionisation (MALDI), mass analysers: Magnetic Sector, Quadrupole, Time of Flight (TOF), Ion Cyclotron Resonance(ICR),detectors: Faraday Cup, Channeltron and Daly detector, resolution, abundance sensitivity, Laser Induced Breakdown Spectroscopy (LIBS), Resonance Ionization Mass Spectroscopy (RIMS) Hyphenated Technique - IC-MS, HPLC-MS, GC-MS.

- **Thermal Methods**

  Principle and applications, Thermogravimetric Analysis (TGA), Derivative Thermogravimetric Analysis (DTG), Differential Thermal Analysis (DTA), Differential Scanning Calorimetry (DSC), Evolved Gas Analysis (EGA)

- **Nuclear Methods**

  Principle of Activation Analysis – Neutron Activation Analysis (NAA), Charged Particle Activation Analysis (CPAA), X-ray fluorescence (XRF) spectrometry: Principles, methodology and matrix effect.

- **Statistics in Chemical Analysis**

  Accuracy, Precision, Errors in quantitative analysis, Classification of errors, Propagation of errors, treatment of errors, Normal distribution, Tests of Significance and Confidence Limits, Reporting of analytical results

- **Laboratory Experiments (Any Five)**

1. Determination of trace impurities in high purity materials by AAS.
2. Application of electroanalytical methods to trace analysis.
3. Anion analysis by ion selective electrode.
4. TGA and DTA study of inorganic compounds
5. Neutron Activation Analysis of trace constituents in a complex matrix
6. Analysis of an alloy sample by EDXRF
7. Chromatographic separation and measurement of the components in a mixture
8. Isotopic Analysis by Mass Spectrometry

Course Outcomes:

- Basic knowledge about various Analytical (spectrochemical, mass spectrometric, thermal, electrochemical and nuclear analytical techniques.
- Theoretical and hands-on experience on the detection and separation tools, used in Analytical Chemistry

References

[1]. Encyclopaedia of Analytical Chemistry: Applications, Theory and Instrumentation, Editor R. A. Meyers, John Wiley & Sons Ltd. (2000).
[2]. Fundamentals of Analytical Chemistry, D.A. Skoog, D. M. West, F. J. Holler, S.R. Crouch, 8th Edition, Thomson (2004).
[3] Principles of Instrumental Analysis, D.A. Skoog, F. J. Holler, T. A. Niemann, 5th Edition, Saunders College Publishing (1998).
[4]. A text book of Quantitative Analysis, A.I. Vogel, 5th Edition Revised by G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, ELBS (1989)
[5] Solvent Extraction of Metals, A. K. De, S. M. Khopkar and R. A. Chalmers, Van Nostrand, Reinhold (1970).
[6] Ion Exchangers, F. Helfferich, McGraw Hill (1962).
[7] Introduction to Modern Liquid Chromatography, L. R. Snyder and J. J. Kirkland, 2nd Edition, Wiley (1979).
[8] High Performance Liquid Chromatography: Principles and Methods in Biotechnology, Editor E. D. Katz, John Wiley and Sons, Chichester (1996)
[9] Atomic Absorption and Emission Spectroscopy, A. Metcalfe, Wiley (1987).
[10] Introduction to Mass Spectrometry: Instrumentation and Techniques, John Roboz, Interscience (1968).
[11] Inductively Coupled Plasma Spectrometry and its Application, Editor Steve J. Hill, Sheffield Academic Press (1998).
[12] Thermal Analysis, T. Daniels, Kogan Page (1973).
[13] Electrochemical Methods, A. J. Bard and L. R. Faulkner, 2nd Edition, Wiley (2001).
[14] Principles of Activation Analysis, P. Kruger, Wiley Interscience (1971).
[15] Principles and Practices of X-Ray Spectrometric Analysis, E. P. Bertin, Plenum Press New York, Fourth Edition (1984).
[16] Statistics and Chemometrics for Analytical Chemistry, J. N. Miller and J. C. Miller, Sixth Edition, Pearson Education Limited (2010).

CY503: Material Science (28 L + 4 P)

Coordinators: Dr. Seemita Banerjee (RPCD)
seemita@barc.gov.in

Course Details:

- **Crystal Structure**

  Different types of unit cells, Space lattices, Miller indices, atomic packings, radius ratio, structures of NaCl, CsCl. ZnS, diamond, CaF2, perovskite, double pervoskites, pyrochlores, spinels, garnet structure and framework solids, aperiodic systems, symmetry, relevance of crystal structures to nuclear materials (glass, ceramics, intermetallics and alloys).

- **Powder X-ray Diffraction Technique for Phase Identification**

  Concept of X-ray diffraction, reciprocal space, Ewald construction, structural and scattering factors, grain/particle size effects, different techniques of recording diffraction patterns, indexing of diffraction patterns, Diffraction data files and their utility, Neutron diffraction, electron diffraction.

- **Types of Bonding in Solids**

  Van der Waals interactions, Lennard-Jones potential, crystals of inert gases, ionic bonding, Madelung energy and its calculation in the case of NaCl/CsCl, covalent bonding, hydrogen bonding.

- **Defects in Solids**

  Defects and defect concentration, dependence on temperature, 0- D, 1- D, 2-D defects, Experimental methods for their characterisation, color centres, phase transitions, classification with examples, dependence of phase transition on T and P, thermodynamic classification of phase transitions, order-disorder phase transitions, austenite- martensite phase transitions in alloys. Solid solutions, their significance, simple and complex solid solutions, methods to characterize solid solutions.

- **Transport Properties of Solids**

  Ionic conductivity, electronic conductivity, dielectric, ferro, piezo and pyro electric materials. structural basis and applications, superconductivity, thermal conductivity with examples.

- **Basic techniques for characterization**

  Concept of various characterization techniques based on X-rays and electrons: XRF, EPMA, XPS, AES, EELS and their application with examples.

- **Methods of material preparation and processing**

  Solid state reactions and soft chemical routes, concepts of annealing, sintering and calcination, processing techniques like spin coating, powder coating, screen printing etc.

- **Laboratory Experiments: (Any two)**

1. XRD characterization, indexing and cell parameter determination
2. Micro structure of metal/alloy by metallography and SEM
3. Electrical resistivity and its temperature dependence

Course Outcomes:

- Fundamental understandings of the Synthesis and characterization, crystal structures, types of bonding and defects in different solid state materials.
- Understanding of the transport properties like ionic and electronic conductivity and the structure-properties correlation for various materials.

References

[1]. Introduction to solid state physics – Charles Kittle
[2] Solid-state chemistry and physics, Vol. 1 & 2 – (Ed) P. F.Weller
[3] A first course in materials science – V. Raghavan
[4] Modern aspects of solid-state chemistry – C.N.R. Rao
[5] New Directions in solid-state chemistry – C.N.R. Rao and J. Gopalakrishnan
[6] Solid-state chemistry and its applications – Anthony R. West
[7] The powder method in X-ray crystallography – Leonid V. Azaroff and M. J. Buerger
[8] Solid-state chemistry techniques (Ed) – A. K. Cheetam and Peter Da
[9] Advanced Techniques for Materials Characterization" Eds. A. K. Tyagi, M. Roy, S. K. Kulshreshtha, S. Banerjee, Trans Tech Publications Ltd, Switzerland (2009)
[10] Functional Materials: Preparation, Processing and Applications, Eds. S. Banerjee and A. K. Tyagi, Elsevier Publishers (2011)
[11] Solid State Chemistry: An Introduction, by Lesley E. Smart, Elaine A. Moore
[12] Principles of the Solid State by H. V. Keer.

CY504: Radiation Detection and Measurements (30 L)

Coordinators: Dr. Dhanadeep Dutta (RCD)
deep@barc.gov.in

Course Details:

- **Interaction of Radiation with Matter**

  - **Interaction of Heavy Charged Particle with matter**
    Ionization in gaseous medium, Bragg's curve, stopping power, Bethe Equation for stopping power, Range of heavy charged particle and straggling, Range energy relationship.

  - **Interaction of Fast Electrons with Matter**
    Comparison with heavy charged particle, LET for electron, Bremsstrahlung radiation, Cerenkov radiation, Bethe Equation, path length and range of electrons, Attenuation and absorption of β particles, Backscattering of β- and Positron annihilation.

  - **Interaction of Electromagnetic Radiations (γ, X-Rays) with Matter**
    Photoelectric Effect, Compton Scattering, Pair Production, Variation of cross section for different process with γ energy and Z of the medium, Attenuation and Absorption of gamma rays

  - **Interaction of neutrons with matter**
    Elastic and Inelastic Scattering of neutrons and slowing down, nuclear reactions

  - **Radiation Detectors**
    Principle of Radiation Detectors: Pulse height spectrum, Counting Characteristics, plateaus, Detection efficiency, Energy resolution, Dead time, Counting Statistics

  - **Gas filled Detectors Ionization Chamber, Proportional counter, GM counter. Scintillation Detectors**
    Organic and Inorganic scintillators, Liquid scintillation counter, Pulse shape discriminator, Solid state scintillation detectors: NaI(TI), CsI and LaBr3 detectors.

  - **Semiconductor Detectors**
    p-n junction, HPGe detector for gamma ray spectroscopy, Clover detectors, Si(Li) for x-ray spectroscopy, Silicon detectors for charged particle spectroscopy.

  - **Neutron Detectors**
    BF3, 3He gas filled counters**.**

- **Solid State Nuclear Track Detectors (SSNTD)**
- **Basic principle and applications**
- **Application of Radiation Detectors in Nuclear Probes**
- **Solid State Nuclear Track Detectors (SSNTD)**
- **Instrumentation for nuclear techniques**

PMT and photo diodes, Single Channel Analyser, ADC, Multi Channel Analyser, basic coincidence circuit, determination of life time using coincidence system, Positron Annihilation Spectroscopy: Instrumentation and Applications, Perturbed angular correlation measurement: Instrumentation and Applications

Course Outcomes:

- Fundamentals of Radiations interaction and their detection applied to various radiation environment.

References

[1] Radiation detection and measurement, G.F. Knoll, John Wiley & Sons

CY505: Nuclear and Radiochemistry (42 L + 6 P) (01-CHEM00-505-F)

Coordinators: Dr. Chhavi Agarwal (RCD)
cagarwal@barc.gov.in

Course Details:

- **Radioactivity**

  Radioactivity, Radioactive decay laws, Half-life and radioactive equilibria.

- **Nuclear Stability**

  Concept of nucleus, Nuclear mass and Binding energy, Nuclear force.

- **Nuclear Models**

  Liquid drop model, Shell model, Concept of spin, Parity electric and magnetic moments, Isomerism.

- **Modes of Decay**

  α decay, β decay, Electron captures, γ de-excitation, Internal conversion.

- **Nuclear reaction and fission**

  Cross-section, Centre of mass system, Compound nucleus, Statistical model, Nuclear fission, Mmass distribution, Heavy ion induced reactions, accelerators, Synthesis of heavy actinides.

  Q value equation, Reaction threshold, Centre of mass system, Cross-section for neutron and charged particle induced reactions, Nuclear Temperature, Compound nucleus mechanism, Nuclear fission: observables and models, Synthesis and separation of heavy and trans-actinides, Accelerators, Application of accelerators in ion beam analysis.

- **Techniques in Nuclear Chemistry**

  Target preparation and target chemistry, Radiochemical separations, Concept of tracer and carrier, Chemical yield, Radiochemical purity, Application of radiotracers in chemical sciences, Determination of half-life.

- **Laboratory Experiments (Any Five)**

1. GM Counter: plateau, statistics and dead time
2. Gamma-ray spectrometry using NaI(Tl) and HPGe detector: Energy Calibration, Resolution,Efficiency
3. Separation of actinides using solvent extraction technique
4. Alpha spectrometry
5. Determination of half-life of a radioisotope
6. Solid State Nuclear Track Detector
7. Separation of fission products / Transient equilibrium

Course Outcomes:

- Provides comprehensive understanding of nuclear structure, stability, and reactions.
- With theoretical and practical training, learners get understating of the radioactive decay processes, nuclear models, fission, synthesis of heavy elements, and radiochemical techniques.

References

[1] Nuclear and Radiochemistry (1981) – G. Friedlander, J. Kennedy, J. M. Miller and J. W. Macias
[2] Atomic Nucleus (1955) - R. D. Evans
[3] Source book of Atomic Energy (1969) - S. Glasstone
[4] Man made elements (1963) - G. T. Seaborg
[5] Essentials of Nuclear Chemistry (1982) - H. J. Arnikar
[6] The Chemistry of Transuranium Elements (1971) - C. Keller
[7] Fundamentals of Radiochemistry, IANCAS Publication, 2007

CY506: Thermodynamics (15 L)

Coordinators: Dr. R.A. Jat (PDD)
avtar@barc.gov.in

Course Details:

- **Introduction to Chemical and Statistical Thermodynamics**

  Laws of thermodynamics, Fundamental equations and thermodynamic potentials, Introduction to statistical thermodynamics, Einstein and Debye theories of specific heats of solids, Phase transitions, Thermodynamics of solutions, ideal and regular solution models

- **Chemical Equilibrium**

  Solid-gas equilibrium, Ellingham diagram.

- **Relation between Thermodynamics and Phase Diagrams**

  Binary and ternary phase diagrams, CALPHAD definition of phases**,** Degree of freedom rule and lever-rule**,** Calculation of simple binary phase diagrams from thermodynamic properties**,** Chemical potential variations across phase diagrams.

- **Phase Diagram and Thermodynamics of Nuclear Fuels**

  Relevant phases for nuclear fuel applications**,** Change in chemical potentials with compositions of virgin fuels**,** Change in chemical potentials with burn-up**,** Thermodynamics of Fuel-Clad and Coolant-Clad interactions, Thermodynamics of molten fluorides, Concepts of metastable materials.

- **Experimental Thermodynamics**

  Calorimetric measurements, Vapor pressure measurements, Estimation of thermodynamic quantities

Course Outcomes:

- Understanding of thermodynamic principles, phase equilibria and thermal analysis techniques enabling application of thermodynamic models to real systems

References

[1] Introduction to Thermodynamics of Materials (Fourth Edition) by D. R. Gaskell (2003) Taylor & Francis Books, Inc., New York
[2] The Principles of Chemical Equilibrium by K. Denbigh (Fourth Edition) (1981) Cambridge University Press, Cambridge
[3] Materials Thermodynamics by Y.A. Chang and W.A. Oates (2010), John Wiley & Sons, Hoboken, New Jersey.
[4] Fundamentals of Classical and Statistical Thermodynamics by B.N. Roy (2002) John Wiley & Sons, Hoboken, New Jersey, England
[5] Comprehensive Nuclear Materials, R.J.M. Konings, T.R. Allen, R.E. Stoller, S. Yamanaka, Elsevier 2012.

CORE COURSES

CY601: Lasers (14 L + 2 P)

Coordinators: Dr. A. K. Singh (HRDD)
aksingh@barc.gov.in

Course Details:

- **Basic principles**

  Spontaneous & stimulated emission, population inversion, laser components, Einstein coefficients, optical amplification, optical & electrical pumping, rate equations (two, three and four level laser systems)

- **Properties of laser beams**

  coherence (spatial and temporal), monochromaticity, intensity, polarization

- **Optical resonators**

  Types, properties, spatial field distribution in resonators, stable & unstable resonators, gain and losses in the cavity, Q-factor, threshold condition, laser modes (longitudinal and transverse)

- **Types & some laser systems**

  Solid state lasers, gas lasers, dye lasers, diode lasers, fiber lasers, free electron laser and quantum cascade lasers, tunable lasers

  Generation of short and ultrashort pulses

  Q-switching and mode locking, chirp pulse amplification

  Non-linear optical techniques

  Phase matching, harmonic generation, optical parametric oscillator & amplifier

  Modulation in laser pulses-amplitude, wavelength, temporal

  Characterization of laser pulses - Measurement of the pulse temporal profile (electronic & optical), spectral measurements (interferometric), amplitude - phase measurements (FROG)

  Laser applications & laser safety.

Course Outcomes:

- Provides an understanding of the generation and manipulation of the laser light through the modules of light-matter interaction, opto-mechanical components of lasers, generation of ultra-short light pulse, frequency conversion and associated nonlinear spectroscopy techniques

References

[1] Laser Spectroscopy: Basic Concepts and Instrumentation- W. Demtroder
[2] Laser Fundamentals-William Silfvast
[3] Laser and Non-linear Optics- B. B. Laud
[4] Principles of Lasers- O. Svelto and D. C. Hanna
[5] Laser Safety- Roy Henderson and Karl Schulmeister

- **Laboratory experiment**

  Time-frequency bandwidth relationship for laser pulses-Checking the Heisenberg uncertainty principle

CY602: Electronics & Chemical Instrumentation (27 L + 6 P)

Coordinators: Shri R. Manimaran (ChD)

Course Details:

- **Electronics**

  DC & AC Fundamentals: Concept of charge, current, voltage, power, Ohms law, AC –Sinusoidal, Peak & RMS values, Frequency.

  Electronic components: Resistors, capacitors, diodes, transformer

  Power Supply, Rectification, Filter, Line/Load Regulation, Regulator Chips, Low Voltage & High Voltage power supplies, SMPS.

- **Analogue Electronics**

  Operational Amplifiers, Ideal Characteristics, Inverting, Non-inverting Amplifier, Integrator, Comparator, Summer, Pulse Amplifier and Instrumentation Amplifier.

- **Digital Electronics**

  Number system and Logic gates - Decimal, Binary and Hexadecimal number systems, Logic gates, Flip Flop, Counter, Decoder, Display Device.

  Analog to Digital Converters and Digital to Analog Converters.

- **Instrumentation**

  Concept of Instrumentation, Order of instruments, concept of broad specifications (accuracy, precision etc), Voltmeter and Current meter, concept of Multimeter & concept of loading.

  Signal & Noise: Concept of Noise & Signal, dB, S/N ratio and improvement techniques.

  Transducers: Transducers and their applications (temperature sensors, PMT, photo diode and vacuum gauges) Signal analysis & Processing: Selective signal amplification, filter, Lock-in-amplification, Boxcar Averager, Fast Fourier Transform.

- **Computer in Labs**

  PCs & interfacing concepts, RS232, USB ports, Embedded systems, Lab View programming.

Course Outcomes:

- Teaches basics of electronics such as various electronic components, power supplies, amplifiers, signal processing, concepts of noise, transducers, safe handling of instruments, PCs and interfacing concepts, etc with an aim to confident handling of the instruments in laboratories

References:
[1] Basic electronics for Scientists- McGraw Hill International (1977) - J. J. Brophy
[2] Basic Electronics - Bernard Grob McGraw Hill Book Co.
[3] Electronic Principles – Tata McGraw Hill Pub. Malvino
[4] Operational Amplifiers and linear integrated circuits –Prentice Hall of India Ltd.-Robert Conghlin, Fredrick Drisco
[5] Art of Electronics, Cambridge University Press, London - Paul Horonitz and Winfield Hill
[6] Digital Principles and applications Tata McGraw Hill - Malvino& Leach
[7] Instrumental methods of chemical analysis, McGraw Hill - Ewing
[8] Introduction to instrumental analysis, McGraw Hill Book Co. - Robert D. Bramn.
[9] Principles of instrumental analysis by Skoog, Holler and Neiman (Fifth Edition)
[10] Electronic Instrumentation & Measurement technique - W D Cooper & A. D. Helfrick
[11] Optimisation of Electronic Measurement - Enke, Croach, &Florlicks
[12] Myer. Kuts, Temperature Control- Wiley (1968)
[13] S. Dushman and J.M. Lafferty- Scientific foundations of vacuum techniques, Wiley (1962)

CY603: Production and Applications of Radioisotopes (30 P)

Coordinators: Dr. Drishty Satpati (RPhD)
drishtys@barc.gov.in

Course Details:

- **Introduction to the course**

  Relevance and contribution of the isotope program in DAE.

- **Production of Radioisotopes**

  - **General introduction on radioisotope production (1 Lecture)**
    Isotopes and radioisotopes, naturally obtained and artificially produced radioisotopes, Need for radioisotope production, Basics of radioisotope production

  - **Production of radioisotopes in a nuclear reactor (3 L)**
    Production of radioisotopes in a nuclear reactor - Various processes, Calculation of activity of radioisotope produced, 'No-carrier-added' and 'carrier-added' radioisotopes, Introduction to Szilard-Chalmer reaction and Bateman equation, Radiochemical processing of the irradiated targets - various techniques, Production routes and radiochemical processing for some important reactor radioisotopes: 60Co, 99Mo, 125I, 131I, 153Sm, 192Ir and 177Lu.

  - **Production of radioisotopes in a cyclotron (2 L)**
    Principles of production of radioisotopes in a cyclotron - Calculation of yield of radioisotopes produced in a cyclotron, Target preparation for production of radioisotopes in a cyclotron, Production and radiochemical separation of some important cyclotron produced radioisotopes: 18F, 44Sc, 64Cu, 68Ge, 89Zr, 123I, 124I, 211At and 225Ac.

  - **Radionuclide generators (2 L)**
    Concept and applications of radionuclide generators, Separation methodologies used in generators, Calculation of elution yield and tmax, Examples of some clinically relevant radionuclide generator systems: 99Mo/99mTc, 68Ge/68Ga, 90Sr/90Y, 188W/188Re, 225Ac/213Bi generators.

- **Applications of Radioisotopes & Radiation in Industry (9 L)**

  - **Radiotracer applications (4 L)**
    Basic principle of radiotracer technology, Advantages of radiotracers, Selection of a radiotracer for a particular study, Injection and Detection of radiotracer, Radiotracer data treatment and analysis, Leak detection, Flow rate measurements, Residence time distribution measurements, Sediment transport investigations, Radiotracer applications in oil fields

  - **Sealed source applications in industry - Principle and applications (1 Lecture)**
    Radiometric measurements, Radiography, Tomography, Nucleonic gauges.

  - **Applications of isotope hydrology (2 L)**
    General principle of hydrology, Measurement techniques, Source and mechanism of recharge, Interconnection between water bodies, Determination of age of ground waters, Pollution studies.

- **Radiation processing applications (2 L)**
  Application of electron beam for processing of materials, Application of gamma radiations for processing of materials.

- **Applications of Radioisotopes & Radiation in Healthcare (13 L)**

  - **Nuclear medicine and radiopharmaceuticals (2 L)**
    Nuclear medicine and its importance in human healthcare, Classification of radiopharmaceuticals, Characteristics of diagnostic and therapeutic radiopharmaceuticals, Mechanism of uptake of radiopharmaceuticals.

  - **Preparation of radiopharmaceuticals (3 L)**
    Design and preparation of radiopharmaceuticals, Methods of radiolabeling, Radiolabeling with Technetium and Rhenium, Radiolabeling using novel cores such as Tricarbonyl, HYNIC, Nitride and '4+1' chemistry, Radiolabeling with Lanthanides, Gallium, Yttrium, Copper etc.

  - **Quality control of radiopharmaceuticals (2 L)**
    Need for quality control of radiopharmaceuticals, Types of quality control tests, Physico-chemical quality control tests, Biological quality control tests.

  - **Nuclear medicine imaging techniques (1 Lecture)**
    Nuclear medicine imaging vs. other contemporary imaging techniques, Concept of tomography, Gamma camera, SPECT, PET and Hybrid imaging (SPECT-CT, PET-CT, SPECT-MRI, PET-MRI), SPECT vs. PET.

  - **Some important radiopharmaceuticals (4 L)**
    Some important organ-specific diagnostic (SPECT as well as PET radiopharmaceuticals) - Contemporary agents for Myocardial imaging, Brain imaging, Renal imaging, Hypoxia imaging, Tumor and inflammation imaging, Infection imaging, Receptor-specific imaging agents etc., Therapeutic radiopharmaceuticals for some specific applications - Bone pain palliation, Radiation synovectomy, Targeted radionuclide therapy, Peptide Receptor Radionuclidic Therapy (PRRT), Radioimmunotherapy (RIT), Targeted Alpha Therapy (TAT).

  - **Concept of thernostics and personalized medicine (1 Lecture)**
    Concept of theranostics, Applications and advantages of theranostics in nuclear medicine, Theranostic radionuclides, Concept of personalized medicine.

Course Outcomes:

- Provides understanding of the production methods of various radioisotopes using nuclear reactor, cyclotron, generator, etc.
- Application of produced radioisotopes in the field of healthcare (radiopharmaceuticals) and industry is taught.
- TSOs gain knowledge about the peaceful uses of atomic energy for the benefit of society.

References

[1] Manual for Reactor Produced Isotopes. IAEA-TECDOC-1340, IAEA, 1999.

[2] Dynamic Mechanical Analysis: A Practical Introduction. K.P. Menars, CRC Press, Boca Raton, 1999.

[3] Industrial application of radioisotopes. G. Foldiak.

[4] Guide Book on Radioisotope Tracers in Industry - Tech. Rep. Series 316, IAEA, Vienna, 1990

[5] Environmental Isotopes in Hydrogeology. Ian Clarke and Peter Fritz, Lewis Publishers, NY, 1997.

[6] Fundamentals of Nuclear Pharmacy, G.B. Saha, Springer-Verlag, 1984.

[7] Radiopharmaceuticals: Chemistry and Pharmacology, Adrian D. Nunn. Marcel Dekker, 1992.

[8] Radiopharmaceuticals: Chemistry and Pharmacology, Adrian D. Nunn. Marcel Dekker, 1992.

[9] PET in Oncology: Basics and Clinical Applications, J. Ruhlmann, P. Oehr, H.J. Biersack. Springer-Verlag, 1998.

[10] Fundamentals of Radiochemistry. D.D. Sood, A.V.R. Reddy, N. Ramamoorthy. Indian Association of Nuclear Chemists and Allied Scientists, 2004

CY604: Reactor Physics and Reactor Chemistry (15 L)

Coordinators: Dr. Drishty Satpati (RPhD)
drishtys@barc.gov.in

Course Details:

- Fission, Energy from fission, Burn-up, Spontaneous and induced fission, Chain reaction, Fissile-Fissionable fertile materials, Prompt and delayed neutrons, Four factor formula, Neutron interaction with matter, Fission products, Critical mass, Neutron Diffusion Theory, Multiplication factor, Reactor kinetics and control.

- Different types of homogeneous and heterogeneous reactors, Components of reactors. Introduction to the types of water-cooled power reactors & their process systems.

- Schemes of preparation of demineralized water, Variation in properties of water and heavy water as a function of temperature and pressure. An overview of types of corrosion, methods of evaluation of corrosion and its prevention. An overview of materials of construction for the different components of reactor systems. Hot Conditioning of PHT circuit in PHWR. An overview of water chemistry regimes in BWR, PWR & PHWR.

- Principles and processes relevant to chemistry control in primary heat transport systems. Radioactivities in reactor waters & their control. CRUD generation and activity transport in the primary heat transport system of reactors its control. Radiolysis of water, related hazard, and its control, Reactivity control through chemistry: Use of soluble neutron poisons- for chemical shim and for emergency shutdown. Purification of reactor cover gas by Catalytic recombination and adsorption techniques.

- Chemistry control in secondary heat transport system, pH control methodologies of secondary system, Scaling and methodology of its control in secondary system.

- Chemistry control in the tertiary heat transport system, Bio-fouling and its control methodologies.

Course Outcomes:

- To impart the foundational understanding of reactor design and operation from a chemist's perspective;
- Reactor Physics component discusses the neutron diffusion theory, reactor dynamics and reactor control;
- Reactor Chemistry component aims on corrosion, the interaction of coolant with reactor structural materials, activity transport, etc.

References

[1] R.A. Knief: Nuclear Energy Technology (1981).
[2] S. Glasstone and M.C. Edlund: The elements of Nuclear Reactor Theory (1952).
[3] P. Cohen: Water Coolant Technology in Power Reactors, American Nuclear Society, U.S.A (1980).
[4] Proc. Int. Conf. on water chemistry in Nuclear Reactor Systems organized by British Nuclear Energy Society, U.K. (1977,1980,1983,1986,1989,1992).
[5] H. H. Uhlig: Corrosion and Corrosion Control, John-Wiley & Sons, N.Y., (1985)
[6] International Atomic Energy Agency, Coolant Technology of Water Cooled Reactors, IAEA-TECDOC-667, Vols. 1-4, Vienna
[7] M. Benedict, T.H. Pigford and Levi: Nuclear Chemical Engineering.
[8] S. Glasstone & A. Sesonske: Nuclear Reactor Engineering, Vol I & II, CBS Publications, Delhi (1977)

CY605: Molecular Structure & Spectroscopy (28 L + 6 P)

Coordinators: Dr. Dimple Dutta (HRDD)
dimpled@barc.gov.in

Course Details:

- **Coordination Chemistry**

  Werner's Coordination theory, Valence Bond Theory, Crystal Field Theory, splitting of "d" orbital in different geometry, Jahn Teller effect, Thermodynamic effects of crystal field, Coordination chemistry of lanthanide and actinide ions, Brief introduction to group theory, Application of group theory for d-d transition, Racah parameters, electronic spectra of complex ions, Tanabe Sugano diagram, nephelauxetic effect, ligand metal orbital overlaps, magnetic properties and susceptibility measurements of complex ions, drawbacks of CFT, f- f transitions in lanthanides.

  Molecular orbital theory and construction of molecular orbital diagram from concepts of group theory, MO's for Sigma bonding in AB6 molecules, tetrahedral AB4 case, MO's for pi bonding in AB6 molecules, Metal organic framework materials. Dissociative & associative reaction mechanism of ligand replacement in octahedral and square planar complexes, trans effect and its implications.

- **Characterization Techniques of Complexes**

  NMR: Basic Principles of NMR Spectroscopy, Chemical Shift, Spin-Spin Coupling, Decoupling Experiments, Pulse NMR, Relaxation Effects, Two-Pulse Experiment, T1-Measurment, T-2 measurement, solid state NMR, ESR: Basic Principles of ESR Spectroscopy, The g-value, Hyperfine Coupling, Electron Nuclear Double Resonance (ENDOR), Mossbauer spectroscopy.

- **Electronic, Vibrational and Rotational Spectroscopy**

  Classification of molecules, their characteristic spectral features and selection rules, pure microwave, Rotational Raman, Vibrational and rotational vibrational spectroscopy, IR and Raman spectroscopy.

  Basic principles of Fourier transform spectroscopy (FTIR, FT-RAMAN).

  Surface enhanced Raman spectroscopy (SERS), Terahertz spectroscopy, Nonlinear optical methods, sum & difference frequency generation (SFG & DFG).

  Synchrotron radiation and its application in spectroscopy, X ray absorption-based techniques (XANES, EXAFS) X ray Photoelectron Spectroscopy.

  Doppler-free high-resolution spectroscopy.

- **Laboratory Experiments**

  Electronic spectra of a transition metal complex. d-d transitions, NMR, FT-IR, Raman

Course Outcomes:

- Understanding of bonding and geometry in coordination compounds through crystal field and molecular orbital theory.
- Interpretation of molecular structure using advanced spectroscopic techniques such as NMR, ESR, and XPS.
- Learners gain insights into electronic, vibrational, and rotational spectroscopy for structural and electronic characterization.
- Overall, it builds analytical skills for correlating spectroscopic data with molecular properties and reactivity via theoretical background and practical experiments.

References

[1] Advance Inorganic Chemistry - F.A.Cotton and G.Wilkinson
[2] Physical Methods in Inorganic Chemistry - R.S. Drago
[3] Modern Coordination Chemistry – Lewis and Wilkins
[4] Introduction to ligand fields - B.N. Figgis
[5] Ligand field theory - C.J. Ballhausen
[6] Comprehensive Inorganic Chemistry - Huchey
[7] Molecular Spectroscopy - C.N. Banwell
[8] Infra red spectra of Inorganic and coordination compounds - K. Nakamoto
[9] Laser spectroscopy: Basic concepts and instrumentation - W. Demtroder

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CY606: Radiation and Photochemistry (28 L + 4 P)

Coordinators: Dr. A. Barik (RPCD)
atanu@barc.gov.in

Course Details:

- **Radiation Chemistry**
  - **Interaction of High-energy Radiation with Matter**
    Chemical consequences, absorption coefficients, G-values, track entities and LET effects, radiation sources. Diffusion kinetics and homogeneous reaction stages, time scales of events in radiation chemistry, ion-pairs, ion-molecule Reactions

  - **Radiation Chemistry of Water and Nonpolar Liquids**
    Radiolysis of water & heavy water, radical and molecular yields, material balance, chemical dosimetry Radiolysis of non-polar solvents, geminate recombination, electron salvation
    Radiation chemistry of micro heterogeneous systems and ionic liquids Comparative aspects of radiolysis of liquids, solids and gases

  - **Experimental Techniques**
    Detection of primary species and free radicals using pulse radiolysis coupled with optical absorption spectroscopy, ESR, conductivity, resonance Raman spectroscopy
    Evaluation of absolute rate constants, pK values of transient species, one-electron redox potentials, picoseconds pulse radiolysis.

  - **Application**
    Radiolytic synthesis of nanoparticles.
    Radiation chemistry of water at high temperature and high pressure. Radiation chemistry of antioxidants and radioprotectors.

- **Photochemistry**

  - **Photophysical Processes**
    Electronic transitions, oscillator strength, selection rules
    Franck-Condon principle, absorption, emission and fluorescence excitation spectra, charge-transfer spectra. Deexcitation processes - fluorescence, phosphorescence, delayed emission,

    triplet-triplet annihilation, heavy atom effect, kinetics of excited state processes, quantum yields of photo-processes. Fluorescence anisotropy
    Photophysical processes in semiconductors, multiphoton processes Environment effect- polarity, viscosity (anisotropy), temperature

  - **Photochemical Processes**
    Excited state acid-base properties, redox potentials, geometry, dipole moments
    Kinetics and mechanism of processes like photo-dissociation, photo-ionization, electron transfer, energy transfer, proton transfer, supra-molecular interactions.

  - **Experimental Techniques**
    Steady-state absorption and fluorescence techniques
    Time-resolved absorption and fluorescence techniques like time-correlated single photon counting, fluorescence up-conversion, nanosecond laser flash photolysis and ultrafast pump-probe spectroscopy; single molecule spectroscopy, fluorescence correlation spectroscopy.

- **Applications**
  Photosynthesis, vision, solar energy conversion, photocatalysis, fluorescence sensors.

- **Laboratory Experiments**

  - **Radiation Chemistry**
    Fricke dosimetry and estimation of G-values.
    Study of free radical reactions using pulse radiolysis technique.

  - **Photochemistry**
    Fluorescence quenching studies: determination of quenching rate constant.
    Excited state properties: determination of acid dissociation constant using absorption & fluorescence techniques.

Course Outcomes:

- Aims on the understanding of the interaction of ionizing and nonionizing radiation with the molecular systems and physico-chemical changes associated with these interactions.

References

- **Radiation Chemistry**

[1] An introduction to Radiation Chemistry. J. W. T. Spinks and R. J. Woods; Wiley Interscience, New York,1990.
[2] Radiation Chemistry: An Introduction. A. J. Swallow; Longman, London, 1973.
[3] Radiation Chemistry. Belloni
[4] Charged particle. A. Mozumdar &Y. Hatano .
[5] Radiation Chemistry: Principles and Applications. Editors: Farhataziz and Michael A. J. Rodgers, VCH,New York, 1987.
[6] The Study of Fast Proccesses and Transient Species by Electron Pulse Radiolysis. Editors: J. H. Baxendale and F. Busi; Reidel, Dordrecht, Holland, 1982.
[7] A. J. Swallow, Reaction of free radicals produced from organic compounds in aqueous solution by means of radiolysis. Prog. React. Kin. 9, 1978, 195.

- **Photochemistry**

[1] K. K. Rohatgi-Mukherjee, Fundamentals of Photochemistry; Wiley Eastern: New Delhi, 1978.
[2] J. B. Birks, Photophysics of Aromatic Molecules. Wiley Interscience, New York, 1970.
[3] J. R. Lakowicz, Principle of fluorescence spectroscopy, 3rd ed.; Springer: New York, 2006.
[4] J. Turro, Modern Molecular Photochemistry, Benzamin, Menlo Park, CA, 1978.
[5] R. P. Wynes, Principles and Applications of Photochemistry. Oxford Science Publications, 1988.
[6] A. Gilbert, J. Baggott, and P. J. Wagner, Essentials of molecular photochemistry, Blackwell Science Inc. Cambridge, USA, 1991.
[7] D. V. O'Connor and D. Phillips, Time Correlated Single Photon Counting. Academic Press, New York (1984).
[8] J. N. Demas, Excited State Life Time Measurements. Academic Press, New York, 1983.

CY607: Chemistry in Nuclear Fuel Cycles (45 P)

Coordinators: Dr. Pranaw Kumar (FCD)
pranaw@barc.gov.in

Course Details:

- Separation and purification of uranium and thorium from their ores, Principles of isotope separation, enrichment of uranium, systematics and processes.
- Conversion processes for preparation of UO2, (U,Pu)O2, UC, (U,Pu)C, UN (U,Pu)N, metals and alloys. Separation and purification of zirconium from its ore, Principle and process for heavy water production. Fuel fabrication processes and chemical quality control.
- Behavior of nuclear fuels (thermal/fast) during irradiation.
- Post irradiation studies, fuel clad chemical interaction, Burn-up etc.
- Thermo-physical and themo-chemical aspects of fuel, Properties of oxide, carbide, nitride and metallic fuel materials, Coated particle based fuels.
- Cladding, moderator, coolant materials and their properties, Liquid metal coolants like sodium and leadbismuth, Chemical aspects of corrosion, Monitoring and maintenance of the purity of coolant.
- Reprocessing of thermal and fast reactor fuels, chemistry of various process PUREX, THOREX etc., Systematic and process of pilot plant CORAL, Challenges in reprocessing of fast reactor fuel.
- Waste processing and management, classification of waste and treatment practices of gaseous, liquid and solid waste.
- Vitrification of high level liquid waste, Partitioning of actinides from high level liquids waste, Decontamination process.
- Nuclear safety, Management of H2, Xe, Kr, I2 and tritium in operating nuclear power plants.

Course Outcomes:

- Fundamental understanding of the chemistry involved in both the front-end and back-end of the nuclear fuel cycle, along with the behavior of fuel during reactor irradiation

References

[1] D. R. Olander: Fundamental Aspects of Nuclear Reactor Fuel Elements: USERDA Report TID-26711(1976)
[2] D. Wilson: The Nuclear Fuel Cycle, From Ore to Waste, Oxford University Press Inc. New York (1996)
[3] E. Glueckauf, Atomic Energy Waste: Its Nature, Treatment and Disposal, Interscience Publishers Inc. NewYork (9161)
[4] R. L. Murray and J. A. Powell: Understanding Radioactive Waste, 4th Edition, Columbus: Battelle Press (1994)

CY608: Advanced Chemical Kinetics & Dynamics (13 L + 4 P)

Coordinators: Dr. P. Mathi (RPCD)
mathip@barc.gov.in

Course Details:

- Intermolecular interaction potential, Collision theory, Potential energy surfaces, Activated complex theory, adiabatic and non-adiabatic reactions, Landau-Zener crossing, Lindemann's theory of unimolecular reactions, energy transfer, fall-off region and its limitations, Hinshelwood's Treatment. Rice-Ramsperger and Kassel (RRK) model, and Marcus refinement of RRK model (RRKM) for the calculation of rate constants of simple unimolecular reactions.

- Molecular beam experiments, types & characteristics of molecular beams, scattering as a probe; differential cross-section; quantum mechanical approach to elastic scattering; conservation of angular momentum – Newton diagram, lab–to-centre of mass transformation, reaction cross section - reaction probability; opacity function – steric factor; reactive asymmetry – angular distribution in reactive collisions – direct reaction versus collision complex; forward, backward, and forward–backward scattering; potential energy contour diagram, reactions with early & late barrier. Different molecular energy transfer processes. Laser based spectroscopic techniques- LIF, REMPI, CRDS, detection and measurement of trace constituents and free radicals, rate coefficient measurement, chemical kinetics and dynamics studies, atmospheric chemistry.

- IR laser chemistry, laser isotope separation, mode and bond selective chemistry, intramolecular vibrational energy redistribution (IVR), coherent control of chemical reaction.

Course Outcomes:

- Provides a comprehensive understanding of reaction rates and molecular mechanisms, enabling them to analyze kinetic data, model reaction pathways, and interpret molecular dynamics for a deeper insight into chemical reactivity and transformation processes.

References

[1] Chemical Kinetics - K. J. Laidler, Third Edition, Pearson Education, Singapore (2004).
[2] Molecular reaction dynamics and chemical reactivity - R. D. Levine and R. B. Bernstein, Oxford University Press, New York (1987).
[3] Chemical dynamics via molecular beam and laser techniques - R. B. Bernstein, Clarendon Press, Oxford (1982)
[4] Unimolecular reactions - P. J. Robinson, S.H. Robertson and K. A. Holbrook, Wiley, London (1996)
[5] Introduction to molecular dynamics and kinetics - G.D.Billing and K.V. Mikkelsen, Wiley, NY (1996)
[6] Chemical Kinetics and Dynamics - J F. Steinfeld, J.S. Francisco and W. L. Hase, Prentice Hall International, Inc. III, New Jersey (1999).
[7] Chemical Kinetics and Reaction Dynamics – P.L. Houston, McGraw-Hill Higher Education, (2001).
[8] Laser Spectroscopy: Basic Concepts and Instrumentation- W. DemtrÖder, Springer International (2004)

CY609: Health Physics and Radiation Biology (15 L)

Coordinators: Dr. B.N. Pandey (RB & HSD)
bnp@barc.gov.in

Course Details:

- **Health Physics**

  - **Fundamentals of Radiation Protection**
    Radioactivity, Ionizing radiation, Radiation quantities and units, Basis and structure of the system for radiation protection, System of radiological protection for human, natural radiation.

  - **Basic Radiation Physics and Radiation Dosimetry Aspects**
    Interaction of radiation with matter, External and internal radiation hazards in nuclear and radiation facilities, Radiation dosimetery: basics, concepts and definitions, External radiation dosimetry and dosimetry of internally deposited radio nuclides, Radiation detection principles, Monitoring instruments and Personnel monitoring devices.

  - **Operational Monitoring and Safety Aspects of Facility Design**
    Exposure situations as per ICRP-103 recommendations, Control of external and internal radiation hazards, Radiation dose limits and its basis, General principles and techniques of radiation monitoring, air activity and area contamination, Assessment and control of radiation hazards in nuclear fuel cycle facilities with special reference to metallurgical, radiochemical and radioisotope facilities and fuel reprocessing plants, Criticality safety aspects, Environmental safety aspects during operation of nuclear and radiation facilities, Industrial hygiene and safety aspects during operation of nuclear and radiation facilities.

  - **Radiological Safety Aspects in Design of Radio-Chemical Laboratories**
    Safety aspects of design of radiochemical laboratory, its types and operational aspects, Partial containment/confinement systems and ventilation system in a laboratory.

  - **Emergency Preparedness and Response System at Nuclear and Radiation Facilities**
    Classification of radiation emergency, Emergency preparedness and response system, Reference levels and guidance values for emergency workers.

  - **Basic Radiation Radiobiology**
    Water radiolysis, Free radicals and its reactions with biological systems, Oxygen effect.
    Radiation damage at bio-molecular level, Damage to DNA and chromosomes (single and double structural breaks, chromosomal aberrations) and its biological consequences, Radiation damage to membrane and its biological consequences, Major health effects of radiation exposure.
    Mode of interaction of different types of radiation with biological systems, Track structure, Concept of LET, Radiobiological effectiveness (RBE), Radiation dose units with reference to radiobiology, Direct and indirect effect of radiation.

  - **Molecular and Cellular Effects of Radiation**
    Assay for radiation damage in human cells (survival curve), Physical and biological factors affecting the cellular radio-sensitivity, Dose and dose rate effect, Dose fractionation, Inverse dose rate effect, Oxygen enhancement ratio and Optimum LET, Radio-protectors and radio-sensitizers.
    Cell cycle arrest and radiation damage repair, Cancer and its induction by radiation, Radiobiology of cancer radiotherapy approaches

Course Outcomes:

- Learners gain foundational knowledge of ionizing and non-ionizing radiation, their properties, and biological effects.
- Develops understanding of cellular responses to radiation, including stochastic and deterministic effects. Applied radiation protection principles (ALARA, time-distance-shielding) and dose limits. Trained in dosimetry, shielding, and monitoring to ensure regulatory compliance.

References

[1] Introduction to Health Physics by Herman Camber
[2] International Commission on Radiological Protection (ICRP) Publication-103, 2007
[3] IAEA- BSS- GSR Part-7, 2015
[4] AERB Safety Guidelines NO. AERB/NRF/SG/EP-5 (Rev. 1), 2015
[5] Biological Effects of Radiation by J. E. Coggle
[6] Radiobiology for Radiologist by Eris J. Hall

CY611: Safety in Chemical and Radiochemical lab (15 L)

Coordinators: Dr. Jaison P.G. (FCD)
jaipg@barc.gov.in

Course Details:

- **Chemical labs**

  Definition of chemical safety and its assessment, general chemical safety awareness, Classification of chemicals: Corrosive, Flammables, explosives, toxics, pyrophoric, carcinogen. Chemical which create lachrymation and smoke, Entry of such chemicals into human/biological system and its consequences, precautionary and safe methods for handling such chemicals, Compatibility issues with chemicals, Understanding the Safety Data Sheets (Material Safety Data Sheets) for different chemicals. Storing different chemicals, incompatible chemicals, making inventory of chemicals, labelling chemicals depending upon its nature, safe disposal of chemicals, precautions and safe operating procedures (SOP) to be taken into consideration for chemical spills, chemical protective clothing, chemical accidents and their classification and consequences, Emergency Procedures during chemical accidents, Personal Protective equipment from chemical exposure, precautions to be taken with chemical which need to be refrigerated. Safe practices while using vacuum lines and laser. Fire safety and different types of fire extinguishers.

- **Radiochemical labs**

  Classification of laboratories, classification of radioactive zones in the laboratory, ventilation, Shielding and dosimetry requirements for handling different types of radioactivity, Radioactivity handling in fume-hoods and glove boxes, Movement of radioactivity within the lab, Washing of radioactive glass wares, Disposal of radioactive aqueous and organic waste, Disposal of compressible and non-compressible radioactive waste, fire safety in radioactive labs, Personnel radiation monitors, Managing personnel and laboratory contamination, Precautions in a radioactive lab and emergency procedures.

Course Outcomes:

- An understanding of the principle of chemical/radiochemical safety.
- The course will make aware about various emergencies and the need of emergency preparedness plans.

ELECTIVE COURSES

CY701: Nanomaterials, Chemical Sensors (15 T)

Coordinators: Dr. B.P. Mandal (ChD)
bpmandal@barc.gov.in

Course Details:

- **An overview of the course**

  - **Physics of nanomaterials**
    Finite size systems, cluster science, bulk versus nanomaterials, quantum confinement effects in nano-regime, evolution of electronic structure from atoms to bulk, density of states, dimensionality and its effect on electronic structure, surface effects, calculation of surface-to-volume ratio for different structural arrangements, size dependent physico-chemical properties, carbon based materials (0D, 1D, 2D and 3D).

  - **Chemistry of nanomaterials**
    Top down and bottom up approaches for synthesis of nanomaterials, such as laser ablation, ball-milling, sputtering, combustion, metathesis, sol-gel etc.

  - **Common characterization techniques for nanomaterials**
    Characterization techniques at different length scales, application of XRD, TEM, SEM, AFM and DLS for characterization of nanomaterials.

  - **Properties of nanomaterials**
    Fundamentals of Semiconductors, direct and indirect band gaps, semiconductor in nano-dimensions (quantum dots, core-shell nano-particles of semiconductors), metallic nanoparticles and surface plasmon, an overview of magnetic, optical and catalytic properties of nanomaterials.

  - **Applications of nanomaterials**
    Nanomaterials in energy conversion (solar cell, rechargeable batteries, supercapacitors and materials for hydrogen energy), nanomaterials for bio-applications (drug delivery), environmental applications (sorbents) and DAE application.

  - **Chemical sensors and their applications**
    Threshold limit values (TLV) of common toxic species, selection of sensor materials mechanism of sensing action, features of sensors (selectivity, response time, reproducibility and regeneration), typical examples of nanomaterials based sensors for H2S, NH3, SO2, and heavy metal ions, common bio-sensors, sensors for DAE applications.

Course Outcomes:

- Idea about different synthesis methods for nanomaterials.
- Knowledge about modern techniques like pulsed laser deposition, spray pyrolysis etc.
- The concepts of Chemical sensors are taught which comprise of various per-requisites of a sensor material.
- Idea about several characterization techniques which are very useful for research work in this area.
- Theory behind the unique properties exhibited by nano-materials help the students to rationally design these materials.

References

[1] Advanced Techniques for Materials Characterization Eds. A. K. Tyagi, M. Roy, S. K. Kulshreshta, S. Banerjee, Trans Tech Publications Ltd, Switzerland (2009)
[2] Fundamental properties of Nanostructured Materials, Eds. D. Fiorani (World Scientific, Singapore, 1994)
[3] Nanostructured Magnetic Materials and their Applications, Eds. D. Shi et al. (Springer, Berlin, 2002)
[4] Mechanical Properties and Deformation Behavior of Materials having Ultrafine Microstructures, Eds. M. Nastasi et al. (Kluwer, Amsterdam, 2002)
[5] Functional Materials: Preparation, Processing and Applications, Eds. S. Banerjee and A. K. Tyagi, Elsevier Publishers (2012).

CY702: Soft Condensed Matters (15 T)

Coordinators: xxxxxxxxx xxxxxxxx

Course Details:

- **Introduction to Soft Matter**

  Forces, energies, length and time scales in soft matter. Soft matter systems (colloids, surfactant / micellar systems, gels, polymer solutions, polymers, polyelectrolytes, microemulsions, membrances, biological macromolecules), Interactions (electrostatic, van der Walls, hydrophilic and hydrophobic interactions, depletion interaction). Viscous, elastic and viscoelastic behavior, Liquids and Glasses, Soft matter in nature

- **Experimental techniques to investigate structure and dynamics in soft matter**

  Scattering techniques (Small-angle X-ray scattering (SAXS), Ultra-small-angle-X-ray scattering (USAXS), Small-angle (SANS) Static and Dynamic light scattering (SLS & DLS).

- **Colloids**

  Introduction, Brownian motion of colloidal particles. Sterically stabilized and Charge stabilized colloids, Colloidal interactions, Liquid phase synthesis of colloidal particles, Structural ordering, Dynamics, Phase Transitions [Gasliquid, Melting /freezing, Glass Transition, Crystal-amorphous].

- **Surfactants**

  Types of surfactants, Micellization, Langmuir- Blodgett films, Monolayer, Bilayers and Vesicles, Lyotropic liquid crystalline phases, Micro emulsions.

- **Polymers and Polyelectrolytes**

  A single ideal chain, mean-squared end to-end distance, radius of gyration. Gaussian chain, Freely joined chain. Excluded volume, solvent quality, theta-temperature. Polymer solutions: Flory-Huggins theory, osmotic pressure, scaling laws for good solvents, Size of a polymer in semi-dilute solutions: osmotic pressure, light scattering, intrinsic viscosity, Classes of gels: physical gels, chemical gels and photo-polymerized gels, Sol-Gel transition, Swelling and shrinking of gels, theory of gelation.

  Polyelectrolytes: Debye-Huckle theory, Donnan equilibrium, manning condensation. Dynamics of polymeric liquids: Maxwell model. Rouse theory, Zimm theory, Reptation theory: tube model, reptation dynamics, self –assembly and order-disorder transitions of diblock copolymers

- **Applications of Soft Matter**

  Nanoparticle suspensions as heat transfer fluids. Colloidal assemblies in liquid-liquid extraction systems. Ionic liquids as extractants. Foams and Gels for decontamination. Foamability of surfactants. Dynamic interfacial tension and foamability. Defoamers, Soft matter in drug delivery and diagnostics.

Course Outcomes:

- Students get to know about the physical basis of soft condensed matter systems.
- Learn interpretation of rheological properties of soft matter with specific examples relevant to pharmaceutical formulations.
- Learn about how to choose appropriate amphiphiles for emulsification.
- Learn about tools for kinetic stabilization of colloidal systems.
- Get an overview of application of soft matter systems in industry.

References

[1] Soft Condensed Matter. R. A. L .Jones, Oxford university (2003)
[2] Soft Matter: Complex Materials on Mesoscopic scales. J.K.G Dhont, G. Gompper and D. Richter (Eds) (Forschungzentrum Jülich GmbH, Jülich-2002)
[3] Ordering and Phase Transitions in Charged Colloids. A.K. Arora and B.V.R. Tata (Eds) (VCH-1996)
[4] Colloidal Dispersions. W.B. Russel, D.A. Saville and W.R. Schowalter (Cambridge university press, Cambridge, 1989)
[5] Intermolecular and Surface Forces. (J.N. Israelachvili) (Academic press, London, 1992)
[6] Micelles. Membranes, Microemulsions and Monolayers. Edited by W.M. Gilbet, A. Ben-Shaul and D. Roux (Springer-Verlag, Berlin,1994)
[7] Principles of Condensed Matter Physics. P.M. Chaikin and T.C. Lubensky, (Cambridge university press, Cambridge, 1995)
[8] Polymer Solutions: An introduction to Physical Properties. Iwao Toraoka, (John Wiley & Sons, 2002)
[9] Polymer Physics. M. Rubinstein and R.C. Colby (Oxford University Press ,2003)
[10] Physical properties of polymeric gels. J.P.C. Added (John Wiley & Sons, 1996).
[11] Neutrons, X-rays and Light: Scattering Methods Applied to Soft condensed matter" P. Linder, T. Zebu Eds. (North Holland-Elsevier, 2002)
[12] Dynamic light scattering: Applications of Photon Correlation Spectroscopy. R. Pecora (Plenum, 1985).
[13] The colloidal domain: where physics, chemistry, biology and technology meet. D. F. Evans and H. Wennerstrom (Wiley-VCH)

CY703: Nuclear Probes for Material Characterization (15 T)

Coordinators: Dr. S.K. Sharma (RCD)
skumars@barc.gov.in

Course Details:

- **Positron Annihilation Spectroscopy**

  Introduction to positron, positronium, formation and its systematic, Experimental techniques, applications in molecular solids, defect studies in metals, alloys and semiconductors, Slow positron accelerators and associated developments in materials characterization.

- **Ion beam analysis**

  Introduction to ion beam analysis, Rutherford backscattering spectrometry, elastic recoil detection analysis, nuclear reactions analysis, particle induced gamma ray emission, particle induced X-ray emission-Theory and applications.

- **Neutron Scattering Techniques**

  Neutron Sources, Properties of Neutron, Neutron Scattering Lengths and Cross-sections, Coherent and Incoherent Neutron Scattering.

- **Small-Angle Neutron Scattering**

  Scattering from General Two Phase Systems, Scattering from Fractal Aggregates, Nuclear vs. Magnetic Scattering

- **Small-Angle Neutron Scattering Instrumentation**

  Experimental Aspects, Data Treatment

- **Analysis of Small-Angle Neutron Scattering Data**

  Model Independent Analysis, Model Dependent Analysis, Contrast Variation

- **Applications**

  Nanomaterials, Colloids, Biological Systems, Porous and Fractal Structures)

- **X-ay absorption Spectroscopy**

  Introduction of X-ray absorption spectroscopy including different processes of absorption of X-rays in materials, Theoretical formalism of EXAFS, Derivation of the EXAFS equation with physical interpretation, Experimental techniques with some introduction to Synchrotron radiation, Data analysis (EXAFS & XANES), Usefulness of the EXAFS technique in material characterization- with few case studies.

Course Outcomes:

- Idea about defects using positron annihilation spectroscopy (PAS).
- Free volume structure characterization of amorphous material using PAS.
- Compositional characterization using Ion beam techniques.
- Phase structure, pore structure, Dynamics, magnetic structure using neutron scattering techniques.
- Analysis of local structure of amorphous and crystalline materials using X-ray absorption methods.

References

[1] Structure Analysis by Small-Angle X-Ray and Neutron Scattering, L.A. Feigin and D.I. Svergun (Plenum Press, New York, 1987)
[2] Neutron, X-Ray and Light Scattering, P. Lindner and T. Zemb (North-Holland, Amsterdam, 1991)
[3] Neutron Scattering from Polymers, J.S. Higgins and H. Benoit (Clarendon, Oxford, 1994)
[4] Analysis of Small-angle Scattering Data from Polymeric and Colloidal Systems: Modelling and Leastsquares Fitting, J. S. Pedersen, Advances in Colloid and Interface Science **70**, 171-201 (1997).
[5] Small-angle Scattering Studies of Biological Macromolecules in Solution, D.I. Svergun and M.H.J. Koch, Reports on Progress in Physics 66, 1735–1782 (2003).

[6] Introduction to XAFS: A Practical Guide to X-ray Absorption Fine Structure Spectroscopy, G. Bunker, Cambridge University Press, 2010.
[7] X-ray Absorption: principles, applications and techniques of EXAFS, SEXAFS and XANES, D.C. Koeningsberger and R. Prins, Wiley (NY) 1988.
[8] Treatise on Heavy Ion Sciences, W.A. Landford, Edited by Allan Bromley, vol. 6, (1986), p363.

CY704: Molecular Bio organics (15 T)

Coordinators: Dr. Dibakar Goswami (BOD)
dibakarg@barc.gov.in

Course Details:

- **New paradigm in synthesis**

  Rational synthetic design, convergent and divergent strategies, multi-component and domino reactions, sequential reactions, high-throughput synthesis, organ catalysis, substrate and reagent controlled asymmetric synthesis

- **New paradigm in synthetic approaches**

  Green strategies, atom economy, bio-catalysis and solvent engineering, microwave and sono-chemistry, nonconventional reaction media (room temperature ionic liquids, super critical fluids, florous phase, super- heated steam), template-driven synthesis.

- **New paradigm in functional targets**

  Design and synthesis of functional molecules/ molecular assemblies, non-covalent interactions, electro- magnetic radiation active organics, organic-inorganic hybrids, organics in nuclear fuel cycles.

Course Outcomes:

- Knowledge about synthetic design, and to enable a student to devise a synthetic route for a target molecule.
- Knowledge about the various strategies in organic synthesis.
- Knowledge about the green strategies, and the know-how of applying the same in organic synthesis.
- Knowledge about the most recent advancements in organic synthesis.
- Knowledge about the use of functional materials used in nuclear fuel cycle in DAE.

References

[1] J. Zhu and H. Bienayme, Multicomponent Reactions, Wiley-VCHVerlaggmbH & Co. 2005.
[2] G. Jung, Combinatorial Chemistry: Synthesis, Analysis, Screening, Wiley, 1999.
[3] W. Bannworth and E. Felder, Combinatorial Chemistry: A Practical Approach, Wiley, 2000.
[4] G. R. Stephenson, Advanced Asymmetric Synthesis, Chapman & Hall, 1996.
[5] P. T. Anastas and T. C. Williamson, Green Chemistry, Oxford Univ. Press, 1998.
[6] C. H. Wong and G. M. Whiteside, Enzymes in Synthetic Organic Chemistry, Pergamon Press 1994.
[7] G. W. Gokel, Advances in Supramolecular Chemistry, 2000.
[8] J. W. Steed and J. L. Altwood, Supramolecular Chemistry, Wiley, 2004.

CY705: Laser Spectroscopy (15 T)

Coordinators: Dr. J.A. Mondal (RPCD)
mondal@barc.gov.in

Course Details:

- **Coherence properties of radiation fields**

  Temporal and spatial coherence, coherence volume, degree of coherence, coherence of atomic systems.

- **Widths and profiles of spectral lines**

  Natural line width, Doppler width, collisional broadening of spectral lines, transit time broadening, homogeneous and inhomogeneous line broadening, spectral line profiles in liquids and solids.

- **Nonlinear optical mixing techniques**

  Phase matching, second harmonic generation, sum frequency and higher harmonic generation, difference frequency generation, optical parametric oscillator and amplifier, tunable Raman laser, Gaussian beams.

- **Spectrometers, interferometers, wavemeters and detectors**

  Basic concepts of spectrometers and interferometers, different kinds of interferometers – Michelson interferometer, Mac-Zhender interferometer, Fabry - Perot interferometer, multilayer dielectric coatings, interference filters, tunable interferometers. Webmeters - Michelson, Sigmameter, Fabry - perot and Feazeu. Detectors – photoconductive and photovoltaic detectors, fast and avalanche photodiodes, photodiode arrays, photomultipliers, multichannel platesand image intensifiers.

- **Absorption and emission spectroscopic techniques**

  High sensitivity methods of absorption spectroscopy - cavity ring down spectroscopy. Laser induced fluorescence spectroscopy, photoacoustic spectroscopy, optothermal spectroscopy, ionization spectroscopy, optogalvanic spectroscopy.

- **Nonlinear spectroscopy**

  Nonlinear absorption, saturation of inhomogeneous line profiles, hole burning spectroscopy, lamb dip spectroscopy, saturation spectroscopy, polarization spectroscopy, multiphoton spectroscopy, Doppler free two photon spectroscopy, saturated interference spectroscopy.

- **Laser Raman spectroscopy**

  Stimulated Raman, coherent anti-Stokes Raman spectroscopy (CARS), Resonance Raman and surface enhanced Raman scattering.

- **Applications of laser spectroscopic techniques in physics, chemistry and biology**

Course Outcomes:

- Skill development in handling high power ultra-short pulsed laser.
- Application of time-resolved and nonlinear laser spectroscopy techniques in chemistry, biology and material science.
- Expertise in indigenous development of novel spectroscopy techniques using Lasers.

CY706: Actinide Chemistry (15 T)

Coordinators: Dr. Sumit Kumar (RACD)
sumitk@barc.gov.in

Course Details:

- **Position in Periodic Table**
  Electronic configuration, The Actinide Concept, Transuranium elements.

- **Actinide Spectroscopy**
  Electronic states, Atomic properties, UV-visible absorption and emission spectroscopy. Time resolved fluorescence spectroscopy (TRFS).

- **Electronic structure and bonding**
  Introduction to 'f ' orbitals and their splitting in the ligand field. Relativistic effect and its consequences. Modern techniques for understanding the bonding in actinide compounds.

- **Co-ordination Chemistry**
  Ionic radii, Coordination number, Hydration Energy.

- **Redox Behavior**
  Redox potentials, Eh-pH diagrams, Variable oxidation states, Ionic species, unusual oxidation states in actinides and their stabilization, Thermodynamic/ kinetics of redox reactions, Disproportionation.

- **Hydrolysis of Actinides**
  Hydrolysis, Polymerization / Depolymerization.

- **Auto-radiolysis**
  Auto-radiolytic effects in aqueous solutions, Auto-radiolysis effects in solid compounds of actinides.

- **Complexation behaviour with inorganic/organic ligands**
  Ion-exchange, Solvent extraction methods for actinides (inter and intra-group separations), Complexation reactions relevant in CQC of nuclear fuels, Analytical chemistry of transplutonium elements, Lanthanides-actinide separation, SANEX process.

- **Actinides in the Environment**
  Natural abundance of actinides, Oklo phenomenon, Actinide speciation in aquatic environment, Complexation with naturally occurring organics such as humic acid and fulvic acid, Sorption and Migration, Interaction with rock, clay, mica etc. Formation and migration of radiocolloids.

- **Biochemistry of Actinides**
  Actinide-microbe interaction, Actinide migration in the food chain, Fixation in human, Pu in blood, Intra-cellular uptake of Pu, Sequestering using chelation therapy, Bioremediation of nuclear wastes.

- **Transactinides**

  Production, Rapid separation techniques, Atom-at-a-time chemistry. Aqueous chemistry of elements 104, 105 and 106

Course Outcomes:

- Understanding of the fuel cycle operations including reprocessing and waste management.
- Idea about environmental aspects of actinide migration in case of accident.
- Pursue further areas of study such as transactinides and 'atom at a time chemistry'.

References

[1] J.J. Kratz, G.T. Seaborg and L.R. Morss; The Chemistry of Actinide Elements, 2nd Edition, Vol. 1&2, Chapman & Hall, New York (1986).
[2] J.J. Katz, L.R. Morss, J.Fuger, and N.M. Edelstein; Chemistry of Actinide and Transactinide Elements, 3rd edition, Springer, Berlin Volume 1-5, (2006).
[3] J.C. Bailar, H.J. Emelius, R. Nyholm and A.F. Trotman-Dickenson; Comprehensive Inorganic Chemistry, Vol. 5, Pergamon Press, Oxford (1973).
[4] A.J. Freeman and C. Keller (Eds.); Handbook of Chemistry and Physics of the Actinides, Vol. 1-6, North Holland Publishers, Amsterdam (1986).
[5] G.R. Choppin and M.K. Khankhasayev; Chemical Separation Technologies and Related Methods of Nuclear Waste Management, Kluwer Academic Publishers, Netherlands (1999).
[6] G.R. Choppin and J. Rydberg; Nuclear Chemistry, Theory and Application, Pergamon Press, Great Britain (1980).

CY707: Computational Chemistry (15 T)

Coordinators: Dr. C. Majumder (ChD)
chimaju@barc.gov.in

Course Details:

- **Introduction**
  Revision to Classical Mechanics, Revision to Quantum Mechanics

- **Force Field Methods**
  Force Field Energy, Stretching, Bending, Out-of-plane bending, Torsion, van der Waals, Electrostatic, cross terms, Validation of Force Fields, Advantage & Limitations.

- **Optimization Techniques**
  Finding Minima-Steepest descent, Conjugate gradient methods, Newton– Raphson methods; Finding Saddle Points-linear and quadratic synchronous transit, gradient norm minimization, Newton–Raphson; Conformational Sampling and the Global Minimum Problem; Stochastic and Monte Carlo methods; Simulated annealing.

- **Electronic Structure Methods**
  Self Consistent Field Theory, Restricted & unrestricted HF, Semi-empirical Methods.

- **Electron Correlation Methods**
  Configuration Interaction Methods, Multi Configuration Self-Consistent Field, Many Body Perturbation Theory, Couple Cluster Method.

- **Basis Sets**
  Slater and Gaussian Type Orbitals, Pople style basis sets, Dunning–Huzinaga basis sets, Correlation consistent basis sets, Plane Wave Basis Functions, Basis Set Superposition Errors.

- **Density Functional Methods**
  Kohn–Sham Theory, Reduced Density Matrix Methods, Exchange– Correlation Functionals-Local Density Approximation, Hybrid or hyper-GGA methods, DFT Problems.

- **Wave Functional analysis**
  Population Analysis Based on Basis Functions, Population Analysis Based on the Electrostatic Potential, Population Analysis Based on the Electron Density, Localized Orbitals, Natural Atomic Orbital and Natural Bond Orbital Analysis.

- **Molecular Properties**
  Perturbation Methods, Derivative Techniques, Electric Field Perturbation, Magnetic Field Perturbation.

- **Simulation Techniques**

  Monte Carlo Methods, Molecular dynamics methods.

- **Computer Laboratory Work**

  Ab initio electronic structure calculation of small systems-designing of input using a visualization program, running an electronic staructure calculation applying GAMESS program, analyzing output manually and using visualization program.

Course Outcomes:

- Calculation of transition state structure and understand reaction mechanism.
- Interpretation of IR and UV-Vis spectra of a system.
- Band structure calculations of solids and analyze results.
- Planning theoretical calculation to explain experimental results and predict molecular properties.
- MD simulation and analysis of simulation results.

References

[1]. An Introduction to Computational Chemistry by Frank Jensen (Wiley)
[2]. Essentials of Computational Chemistry: Theories and Models by Christopher J. Cramer (Wiley)
[3]. Electronic Structure: Basic Theory and Practical Methods by Richard M. Martin. (Cambridge University Press)
[4]. Molecular Quantum mechanics by Atkins & Friedman [5]. Computer Simulation of Liquids by Allen & Tildesley.
[5] Computer Simulation of Liquids by Allen & Tildesley

CY708: Advanced NMR Spectroscopy (15 T)

Coordinators: Dr. Sandeep Dey (ChD)
dsandip@barc.gov.in

Course Details:

- **The basics of NMR experiment**

  Basics of NMR spectroscopy, Pulse NMR, The mechanisms of relaxation, The components of a modern NMR instrument, Basic data acquisition and processing.

- **The NMR of Important Nuclei**

  Chemical shifts for 1H, 13C and 31P nuclei, Homolnuclear and heteronuclear couplings (J), Factors that influence the sign and magnitude of J.

- **Double Resonance Techniques and Complex pulse sequences**

  Decoupling experiments (homonuclear and heteronuclear), Nuclear Overhauser Effect (NOE), Distortionless Enhancement by Polarization Transfer (DEPT) Experiments.

- **The study of dynamic processes by NMR**

  Reversible and irreversible dynamic processes, Reversible complexation and chemical shift reagents, Variable temperature NMR, Determination of activation parameters.

- **Two-Dimensional NMR Spectroscopy**

  Basics of 2D NMR experiments, 1H-1H Correlation Spectroscopy, 1H-13C Correlaion Spectroscopy.

- **Nuclear magnetic resonance in solids**

  Basic NMR interactions in the solid state and their relative magnitudes, Chemical shift tensors and their orientation, Dipolar and quadrupolar couplings, Electron Paramagnetic effects in solid state NMR, Differences in the solid state NMR spectra from spin ½ and quadruple nuclei, Detection of NMR signals in solids, Wide line and zero field NMR experiments.

- **High resolution Solid State NMR experiments**

  Magic Angle Spinning (MAS) NMR experiments, Side band manipulations and line shape analysis in MAS NMR experiments, Evaluation of chemical shift anisotropy parameters form side band intensity analysis, Cross Polarization Magic Angle Spinning (CP MAS) NMR experiments with suitable examples, Probing the local environment around nuclei and measurement of inter-nuclear distances by different solid state NMR techniques, Variable temperature MAS NMR experiments, Multi Quantum (MQ) MAS NMR experiments, Application of solid state NMR techniques for characterization of glasses, porous and amorphous materials, polymers, biomaterials, nano-materials, hybrid-materials, catalysts etc.

- **Principle of NMR imaging**

Course Outcomes:

- Student can learn how to validate the experimental results of synthesis and purity in a fast and efficient way.
- Determination of solution structure with the help of 1H and multi-nuclear NMR spectra.
- Student can analyze the inter-molecular interactions and dynamics in solution state.
- Familiarise the student to use solid state NMR technique for solving problems in Materials science.

References:

[1] Understanding NMR Spectroscopy, 2nd Edition, James Keeler, Wiley, 2008
[2] Becker Edwin D., High Resolution NMR: Theory and Chemical Applications, 3rd Edition, Academic Press 1999.
[3] A complete introduction to modern NMR spectroscopy, R. S. Macomber, Wiley Interscience, 1998.
[4] Sanders, Jeremy K. M. and Brian K. Hunter. Modern NMR spectroscopy: a guide for chemists, Oxford; New York: Oxford University Press, 1987.
[5] Solid state NMR in Materials Science: Principles and Applications By Vladimir I. Bakhmutov, CRC Press, Boca Raton (2012)
[6] C. A. Fyfe, Solid State NMR for Chemists, CFC press, Guelph (1983)

CY709: Atmospheric Chemistry (15 T)

Coordinators: Dr. P. Mathi (RPCD)
mathip@barc.gov.in

Course Details:

- **Structure of Atmosphere**
  Physical characteristics, Chemical Composition, Carbon, Hydrogen and oxygen cycle.

- **Atmospheric Radiation**
  Terrestrial and solar radiation, Energy balance for Earth and Atmosphere, Radiative flux, Actinic flux; Spectroscopy, Absorption of radiation by atmospheric gases and aerosols, Absorption by O2 and O3, Radiative forcing, Photolysis rate as a function of altitude.

- **Chemistry of Troposphere and Stratosphere**
  Stratosphere - Chapman mechanism - HOx, NOx cycle Troposphere - Hydroxyl radicals and other tropospheric oxidants, Photochemical cycles of NO2, NO and O3, Chemistry of NOx, carbon monoxide, Methane, Definition of tropospheric lifetimes, Importance of gas phase kinetics.

- **Atmosphere Pollutants**
  Oxides of nitrogen, Volatile Organic Compounds (VOCs), Halogenated compounds, Sulfur compounds and particulate matter.

- **Effects of pollution**
  Photochemical smog - production of ozone and NOx; trends in trophospheric ozone concentration, relationship of VOCs and NOx to O3, atmospheric chemistry of ozone and its precursors, chemistry of sulfur and nitrogen compounds, Acid Deposition.

- **Global effects of pollution**
  Green House Effect, Global Warming Potential, Stratospheric Ozone Depletion, Ozone depletion Potential, Montreal / Kyoto protocol.

- **Laboratory and field measurements**
  Techniques for species identification and quantification, Aerosoles - formation, sampling and characterization. Experimental methods to study reactions of importance in the atmosphere (Laser Induced Fluorescence, Chemiluminescence, Cavity Ring Down Spectroscopy).

Course Outcomes:

- Idea about structure of atmosphere and atmospheric radiation.
- Knowledge about various photochemical cycles.
- Knowledge about various atmospheric pollutants and their harmful effects.
- Idea about experimental methods to study reactions of importance in the atmosphere.

References

[1] Introduction to Atmospheric Chemistry, D.J. Jacob, Princeton University Press, 1999.
[2] Atmospheric Chemistry and Physics, from Air Pollution to Climate Change, J.H. Seinfeld and S.N. Pandis, Wiley-Interscience.
[3] Introduction to Atmospheric Chemistry, P.V. Hobbs, Cambridge University Press, 2000.
[4] Chemistry of the Upper and Lower Atmosphere, Finlayson-Pitts and Pitts, Academic Press.
[5] Atmospheric Chemistry, A.M.Holloway and R.P.Wayne, RSC Publishing.
[6] Chemistryof Atmospheres, R. P.Wayne, Oxford University Press, 1991.

CY710: Statistical Analysis (15 T)

Coordinators: Dr. K.K. Swain (ACD)
kallola@barc.gov.in

Course Details:

- Population and Sample, Treatment of data, Frequency distribution, Measure of central tendency, Measure of variability, Probability distribution, Probability, Discrete distribution, Continuous distribution, Sampling theory, Sampling distribution, Sampling distribution of means, Statistical inference, Test of hypothesis and significance, One tailed and two tailed tests, Type I and type II errors, Operating characteristic curves and power of a test, Sampling distribution of variance, F distribution, Chi-square distribution, Curve fitting, The method of least squares, Regression, Correlation theory, Linear correlation, Multiple correlation, Analysis of variance, One-way ANOVA, Two-way ANOVA, Factorial designs.

Course Outcomes:

- Knowledge of various terminologies used in Statistics.
- Understanding of various statistical tools which can help in decision making.
- Ways to improve quality in analytical data.
- Proper way of representing analytical data.

References

[1] Murray R Spiegel, Statistics: Schaum's outline series
[2] F. J. Dixon and W. J. Massey, Introduction to statistical analysis
[3] S. N. Deming and S. L. Morgan, Experimental Design: A chemometric approach
[4] Zivorad R. Lazic, Design of experiments in chemical Engineering
[5] J. N. Miller, J. C. Miller, Statistics and chemometrics for analytical chemistry, Sixth edition

NON-SUBJECT ASSIGNMENTS

CY591: Viva Voce (4 Credit, 200 Marks)

Course Details:

In addition to the formal assessment carried out by the method of written examinations, a viva voce examination is also conducted in each semester. The objective of the examination is to assess the grasp of the basic concepts in the courses covered and also to examine the aptitude of the student to apply the knowledge gained in individual subjects to establish linkages and solve problems across domains.

Course Outcomes:

- To evaluate the understanding of subject.
- To judge the thinking process.

CY592: Mini Project (270 Lecture)

Course Details:

The 11 week Mini-Project is prescribed as an integral part of the training school curriculum. It is carried out in the third trimester on completion of the foundation and core courses. The principle objective of carrying out a Mini- Project is to provide a hands-on experience to the trainee of working in an ongoing project of the Department. If feasible, the Mini- Project is linked to the M.Tech. Project and the future work profile of the trainee, thus providing a meaningful synergy between the training, M Tech Project and work profile of the trainee. The experience gained in formulating and executing a scientific/technical problem and the possible pathways to its solution serves as value addition to the training provided. Interactions with senior scientists/ technologists during the project work provide useful insights into the methodologies of research, development and deployment adopted by the BARC scientists and technologists. The trainee compiles a project report highlighting the scope, methods and deliverables of the project followed by a seminar presentation to an expert committee of the work carried out. The Mini-Project carries a weightage of 300 Marks, 225 being awarded by the expert committee and 75 by the guide.

Course Outcomes:

- Idea about how to do literature survey on a given topic.
- Idea about planning and execution of an experiment.
- Data analysis.
- Writing project report.
- Presentation of data and results.

CY593: Seminar (4 Credit, 200 Marks)

Course Details:

As a part of the course curriculum, all trainees have to make a seminar presentation. For this purpose, the trainee is asked to choose a topic of presentation based upon his/her aptitude and area of research interest. The objective of this exercise is to inculcate skills in the trainee on aspects such as analysis of the experimental data, details discussion on the results and hypothesis presented and drawing of meaningful conclusions. A Seminar Committee constituted for this purpose evaluates the presentation based upon attributes such as scientific content, quality of presentation and ability of the trainee to defend the subject of presentation. A maximum of 200 marks have been allocated for the seminar.

Course Outcomes:

- Idea about how to do literature survey on a given topic.
- Dissemination of information available in literature.
- Practical experience of preparing presentation slides.
- Practical experience of discussing scientific results in front of a knowledgeable audience.