Biju Patnaik University of Technology, Odisha
Two-Year (Semester System & Credit system) M. Sc. program
M.Sc. in Applied Chemistry

New Syllabus will be implemented from 2016-17 onwards.

PREAMBLE:

Duration – 2 year full-time course
Total No. of Semester – 4 (Two semesters per year)
Total No. of Theory Papers – 20 (each theory paper of 3 to 4 credit)
Total No. of Practical course – 8 (each practical paper of 2 to 3 credit)

No. of papers (theory) per semester – 4 / 5

No. of practical course per semester – 2 / 3

Grading System- 9 point credit system (2-10) with Maximum 10

DISTRIBUTION OF MARKS

Subject type	**Total points**	**Class tests**	**End semester examination**	**Pass points**
Theory papers (core, allied elective and free elective)	100	2 class tests of 15% points each	70 % points	25 out of 70 & 12 out of 30
Practical/Laboratory	100	Minimum 10 experiments @ 10 % points	-	50% points
Project	100	-	-	50 % points
Seminar	100	-	-	50 % points

Minimum Credit Requirement for Award of Degree: 100

ELGIBILITY FOE ADMISSION:

+3 Sc. preferably Chemistry honors, passed out students

MEDIUM OF INSTRUCTION: English

STRUCTURE OF SYLLABUS

Semester - I

Subject type	Subject code	Subject name	L-T-P	Credit
Theory	MCYC101	Inorganic Chemistry-I	3-1-0	4
Theory	MCYC102	Organic Chemistry-I	3-1-0	4
Theory	MCYC103	Physical Chemistry-I	3-0-0	3
Allied Elective	MCYE104	Quantum Chemistry & Group Theory	3-1-0	4
Allied Elective	MCYE105	Molecular Spectroscopy	3-0-0	3
Practical	MCYC150	Inorganic Chemistry –I Laboratory	0-0-6	3
Practical	MCYC151	Organic Chemistry Laboratory	0-0-6	3
		Total	**30**	**24**

Semester - II

Subject type	Subject code	Subject name	L-T-P	Credit
Theory	MCYC201	Inorganic Chemistry-II	3-1-0	4
Theory	MCYC202	Organic Chemistry-II	3-1-0	4
Theory	MCYC203	Physical Chemistry-II	3-0-0	3
Allied Elective	MCYE204	Spectroscopic Identification of Molecules	3-1-0	4
Free Elective	MCYF205	Chemical Biology	3-0-0	3
Practical	MCYC250	Inorganic Chemistry- II Laboratory	0-0-6	3
Practical	MCYC251	Physical Chemistry-I Laboratory	0-0-3	2
Practical	MCYF252	Computational Chemistry Laboratory	0-0-6	3
		Total	**33**	**26**

Semester - III

Subject type	Subject code	Subject name	L-T-P	Credit
Theory	MCYC301	Analytical Techniques – I	3-0-0	3
Theory	MCYC302	Organic Chemistry-III	3-0-0	3
Free Elective	MCYF303	Environmental Chemistry	3-1-0	4
Free Elective	MCYF304	Materials Chemistry	3-0-0	3
Free Elective	MCYF305	Solid State Chemistry	3-0-0	3
Practical	MCYC350	Physical Chemistry –II Laboratory	0-0-6	3
Practical	MCYF351	Environmental Chemistry Laboratory	0-0-3	2
Practical	MCYF352	Chemical Biology Laboratory	0-0-3	2
	MCYC-314	Seminar	0-0-3	2
		Total		**25**

Semester - IV

Subject type	Subject code	Subject name	L-T-P	Credit
Theory	MCYC401	Analytical Techniques – II	3-0-0	3
Theory	MCYC402	Polymer Chemistry	3-1-0	4
Free Elective	-	Elective-I	3-1-0	4
Free Elective	-	Elective-II	3-1-0	4
	MCYC450	Project	0-0-15	10
		Total		25

25

Choose one paper from each group of Elective-I and II

Group	**Elective – I**	**Elective - II**
Group-A	MCYF 403- Pharmaceutical Chemistry-I	MCYF 404- Pharmaceutical Chemistry-II
Group-B	MCYF 405- Synthesis and Characterization of Materials	MCYF 406- Advanced and Functional Materials
Group-C	MCYF 407- Chemistry of Natural Products	MCYF 408- Supramolecular Chemistry **or** MCYF 409- Nuclear Chemistry

Subject Code – details

M – Master programme
CY- Chemistry
C – Core papers
E- Allied Elective
F- Free Elective
1st Digit – Semester number
2nd & 3rd digits – running number of the papers
(01 to 10 for theory papers. 50 and above for practicals)

1st Semester

MCYC101 INORGANIC CHEMISTRY (3-1-0) 4 credits

Module I

Stereochemistry and Bonding in Main Group Compounds

VSEPR, Walsh diagrams, dπ-pπ bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

Metal - Ligand Bonding

Limitations of CFT, MOT: sigma bonding and energy level diagram in octahedral, tetrahedral and square planar complexes; pi-bonding and energy level diagram in octahedral complexes, angular overlap model.

Module II

Electronic Spectra of Coordination Compounds

Spectroscopic ground states, term symbols for d^n ions, Racah parameters, selection rules and intensities of bands, Orgel diagram, correlation and Tanaube-Sugano diagrams, spectra of 3d metal-aqua complexes of trivalent metal ions (d^1-d^6), divalent Mn, Co and Ni, $CoCl_4^{2-}$, calculation of Dq, B and β parameters, CT spectra.

Spectral properties of lanthanide and actinide metal complexes.

Module III

Metal-ligand Equilibria in Solution

Stability of metal complexes, Stepwise and overall stability constant, factors affecting the stability constant, determination of stability constants and their applications, compositions of metal complexes by Job's method..

Inorganic Reaction Mechanism

Reactivity of metal complexes, inert and labile complexes, factors affecting the reactivity of complexes, mechanisms of substitution (acid, base and anation) reactions of octahedral complexes, isotope effects, Berry's pseudo rotation, Swain-Scott equation, substitution reactions of square planar complexes, trans-effect – theories and applications in synthesis of metal complexes, Redox reactions: mechanism of one election transfer reaction (inner sphere and outer-sphere), Marcus theory for outer-sphere reactions.

Selected Text/Reference Books:

1. D. F. Shriver, P. W. Atkins, *Inorganic Chemistry,* 3rd Edn., Oxford University, Oxford, 1999.
2. N. N. Greenwood, A. Earnshaw, *Chemistry of the Elements,* Pergamon Press, 2nd Edn., 2002.
3. B. Douglas, D. McDaniel, and J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., John Wiley, New York. 1993
4. D. Katakis, and G. Gordon, *Mechanism of Inorganic Reactions*, John Wiley & Sons: N. Y (1987).
5. J. E. Huheey, E. A. Keiter, R. L. Keiter & O. K. Medhi, *Principles of Structure and Reactivity (1st impression)*, Pearson Education, 2006.
6. F. Basolo & R. G. Pearson, *Mechanism of Inorganic Reactions*, Wiley Eastern, 1967.
7. F. A. Cotton, G. Wilkinson, C. A. Murillo & M. Bochmann, *Advanced Inorganic Chemistry,* 6th Edn, John Wiley, 1999.
8. R. G. Wilkins, *The Study of Kinetics and Mechanism of Reactions of Transition Metal Complexes,* Allyn & Bacon, Boston, 1974.
9. Robert B. Jordan, *Reaction Mechanisms of Inorganic and Organometallic Systems,* Oxford University Press, 1998.
10. A.K. Das and M. Das, *Fundamental Concept of Inorganic Chemistry,* Vol. 4 and 5, CBS Publisher & Distributor Pvt. Ltd., New Delhi, 2014.

MCYC 102 ORGANIC CHEMISTRY-I (3-1-0) 4 Credits

Module I (14 hours)

Nature of Bonding in Organic Molecules:

Delocalised chemical bonding conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerenes, tautomerism.

Armaticity in benzenoid and nonbenzenoid compounds, alternant and non-alternant hydrocarbons.

Huckels rule, energy level of π- molecular orbitals, annulenes, antiaromaticity, Ψ-aromaticity, homo-aromaticity, PMO approach.

Bonds weaker than covalent, addition compounds, crown ether complexes and cryptands, inclusion

compounds (cyclodextrins, catenanes and rotaxanes).

Stereochemistry:

Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding.

Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution.

Optical purity, enantiotropic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis.

Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape.

Module II (12 hours)

Reaction Mechanism (Structure, Reactivity and Rearrangements):

Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes.

Types of mechanisms: S_N2, S_N1, mixed S_N1 and S_N2 and SET, S_E1.

Kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, potential energy diagrams, transition states and intermediates.

Methods of determining reaction mechanisms, isotope effects.

Hard and soft acids and bases concept and its application in organic synthesis.

Effect of structure on reactivity: resonance and field effects, steric effect.

Quantitative treatment, Hammet equation and linear free energy relationships, substituent and reaction constants, Taft equation.

The NGP mechanism, NGP by π and σ bonds, anchimeric assistance.

Classical and nonclassical carbocations, phenonium ions, norbornyl systems, common carbocation rearrangements.

The S_N1 mechanism, SN at an allylic, aliphatic trigonal and a vinyl carbon.

Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultra sound, ambient nucleophile and regioselectivity.

Module III (14 hours)

Aromatic Electrophilic Substitution Reactions:

The arenium ion mechanism, orientation and reactivity, energy profile diagrams, the ortho/para ratio, ipso attack, orientation in other ring systems, quantitative treatment of reactivity in substrates and electrophiles, diazonium coupling, Vilsmer reaction, Gattermann-Koch reaction.

The SNAr, S_N1, benzyne $S_{RN}1$ mechanisms, reactivity effect of substrate structure, leaving group and attacking nucleophile.

The von Richter, Sommelet-Hauser and Smiles rearrengements.

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance, reactivity of aliphatic and aromatic substrates at bridgehead, reactivity in the attacking radicals, effects of solvents on reactivity.

Text Books:

1. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, Michael B. Smith, 7th Edition, Wiley, 2013.
2. Advanced Organic Chemistry Part A: Structure and Mechanisms, Carey, Francis A., Sundberg, Richard J, Fifth Edition, Springer International Edition, 2007.

Reference Books:

1. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Sixth Edition, John Wiley & Sons, Inc., New York,1985.
2. Structure and mechanism in organic chemistry, von C. K. Ingold. Cornell Univ. Press, Ithaca. 1953
3. Organic Chemistry, R. T. Moririson and R. N. Boyd, Sixth Edtion, Prentice-Hall, 1992.
4. Modern Organic Reactions, H. O. House, Benjamin-Cummings Publishing Co.,Subs. of Addison Wesley Longman,US;2nd edn, 1972..
5. Principles of Organic Synthesis, R. O. C. Norman and J.M.Coxon, Third Edition, Blackie Academic and Professional, 1993.
6. Pericyclic Reactions: A Mechanistic Study.S. M. Mukherji Macmillan India Press, New Delhi, ,1979.
7. Reaction Mechanism in Organic Chemistry, S. M. Mukherjii and S. P. Singh, Third Edition Macmillan India Press, New Delhi, 1976.
8. Stereochemistry of Organic Compounds. D. Nasipuri,Third Edition, New Age International, 2014.
9. Stereochemistry of Organic Compounds. P.S.Kalsi, Eighth Edition, New Age International, 2015.
10. Organic Synthesis: Clayden J., Greeves N, Warren S, and Wouthers, Second Edition Oxford University Press, 2000.

MCYC103 Physical Chemistry-I (3-0-0) (3 credits)

Module I (10 hours)

Thermodynamics: A brief survey of laws of thermodynamics.

Standard States for Gases, Liquids and Solids and its Applications. Free Energies, Enthalpies and Entropies of Ions in Solutions. Activity and Mean Activity Coefficients of Electrolytes and their Determinations, Debye-Huckel Limiting Law. Thermodynamics of Mixing–Mixtures of Volatile Liquids– ideal and Real Solutions and Activities-Excess Functions. Thermodynamic Derivations of Phase Rule, Applications to two component(eutectic)and three component systems involving solids and liquids (Acetic Acid – Chloroform - Water, NaCl-Na_2SO_4-H_2O, NH_4NO_3-$(NH_4)_2SO_4$-H_2O.

Module II (8 hours)

Statistical Thermodynamics: The Boltzman equation, most probable configuration and concept of residual entropy. The Boltzman distribution formula.

The concept of partition function, Molecular partition functions: translational, rotational, vibrational and electronic partition functions. Characteristic temperatures, Translational partition function of a mono-atomic gas and derivation of ideal gas equation. Principle of equipartition of energy.

Module III (10 hours)

Electrochemistry-I: Debye Huckel-Onsager equation for the equivalent conductivity of electrolytes – experimental verification of the equation –conductivity at high field and at high frequency –conductivity of non aqueous solutions-effect of ion association on conductivity. The electrode-electrolyte interface-electrical double layer-electro capillary phenomena- Lippmann equation–the Helmholz–Perrin–Guoy-Chapmann and Stern models, Electrokinetic phenomena Tiselius method of separation of proteins - membrane potential.

Module IV (8 hours)

Electrochemistry-II: Elecrodics - Mechanism of electrode reactions-polarization and overpotential –The Butler volmer equation for one step and multistep electron transfer reaction– significance of equilibrium exchange current density and symmetry factor- significance of transfer coefficient-mechanism of the hydrogen evolution reaction and oxygen evolution reactions. Some electrochemical reactions of technological interest-corrosion and passivity of metals-construction and use of Pourbaix and Evans diagrams- methods of protection of metals from corrosion, Fuel cells - electro deposition.

Text Books

1. S. Glasstone, Thermodynamics for Chemists, Affiliated East West Press, 1965.
2. D. A. McQuarrie and J. D. Simon, Physical Chemistry: A Molecular Approach,Viva Student Edition,2015.
3. R. J. Silbey, R. A. Alberty, M. G. Bawendi, Physical Chemistry, Wiley, 4th Edition, 2005.

References

1. J. O. M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Plenum Press, 1970.
2. P.W. Atkins, Physical Chemistry, 8th Edn., Oxford University Press, 1998.
3. J. Rajaram and J. C. Kuriacose, Thermodynamics for Students of Chemistry, Shobanlal Nagin Chand Co, 1986.

MCYE104 QUANTUM CHEMISTRY AND GROUP THEORY (3-1-0) (4 credits)

Module-I (12 hours)

Quantum Chemistry-I: Operators in Quantum mechanics: Linear, Hermitian and Angular Momentum operators, Eigenvalue problem.

Basic postulates of quantum mechanics. The Schrodinger equation, Particle in 1,2 and 3-dimensional boxes, degeneracy.

Module-II (8 hours)

Quantum Chemistry-II: Harmonic oscillator, Spherical Coordinates: Rigid rotator, Solution of the Schrodinger equation for Hydrogen like atoms, Significance of n, l and m quantum numbers. Linear Variation and Perturbation Methods. Multielectron atoms, spin quantum number, Ground and excited state of helium atom.

Module-III (10hours)

Quantum Chemistry-III: Hydrogen Molecule ion, Born-Oppenheimer approximation, LCAO-MO approximation, Hydrogen Molecule, Valence Bond and Molecular Orbital Theory. Homonuclear and heternuclear diatomic molecules (HF, CO, NO)

Module-IV (10 hours)

Group Theory: Symmetry Elements and Symmetry Operations, Point Groups, Representation of Groups, Reducible and Irreducible Representation; Character Tables, Applications of Great Orthogonality Theorem.

Text Books (Quantum Chemistry and Group Theory)

1. D. A. McQuarrie and J. D. Simon, Physical Chemistry: A Molecular Approach,Viva Student Edition,2015.
2. D. A. McQuarrie, Quantum Chemistry,Viva Student Edition,2015.
3. M. S. Gopinathan and V. Ramakrishnan, Group Theory in Chemistry, Vishal Publishers,1988.
4. Cotton, F. A. Chemical Applications of Group Theory, 3rd Edn., John Wiley and Sons, 2003.

Reference Books

1. N. Levine, 'Quantum Chemistry', 4th Edn., Prentice Hall India, 2001.
2. A. K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill, 1994.
3. Jack Simons, Introduction to Theoretical Chemistry, Cambridge University Press, 2003.
4. P. W. Atkins. Molecular Quantum Mechanics, Oxford University Press (1986).

MCYE105 MOLECULAR SPECTROSCOPY (3-0-0) (3 credits)

Module I (8 hours)

Basic elements of spectroscopy, Interaction of Radiation with matter, Time dependent perturbation. Einstein coefficients. Integrated absorption coefficients. Transition dipole moments and general selection rules based on symmetry ideas.

Atomic spectra: Characterization of atomic states. Microstate and spin factoring methods. Hund's rules. Derivation of spin and orbital selection rules (based on recursion relations of Legandre polynomials). Spectra of complex atoms. Zeeman and Stark effects.

Module II (8 hours)

Introduction to molecular spectroscopy: Rotational spectroscopy of diatomic molecules. Rigid rotor approximation. Determination of bond lengths and/ or atomic masses from microwave spectral data. Effect of isotopic substitution. Non-rigid rotator. Classification of polyatomic molecules. Energy levels and spectra of symmetric top molecules and asymmetric top molecules.

Vibrational spectroscopy: Homonuclear and heteronuclear diatomic molecules. Extension to polyatomic linear molecules. Derivation of selection rules for diatomic molecules based on Harmonic oscillator approximation. Force constants and amplitudes. Anharmonic oscillator. Overtones and combination bands.

Dissociation energies from vibrational spectral data. Vibration-rotation spectra, P, Q and R branches. Breakdown of the Born-Oppenheimer approximation.

Module III (8 hours)

Raman spectroscopy: Stokes and anti-Stokes lines. Polarizability of molecules. Rotational and Vibrational Raman spectroscopy. Selection rules. Polarization of Raman lines.

Electronic spectroscopy: Diatomic molecules. Selection rules. Breakdown of selection rules. Franck-Condon factors. Dissociation energies. Photoelectron spectroscopy of diatomic (N_2) and simple polyatomic molecules (H_2O, formaldehyde). Adiabatic and vertical ionization energies. Koopmans' theorem.

Module IV (10 hours)

NMR: General introduction and definition; chemical shift; spin –spin interaction; shielding mechanism of measurement; chemical shift, Karplus curve, variation of coupling constant with dihedral angle.

Electron Spin Resonance: Electron spin and Magnetic moment , Resonance condition in ESR and significance of 'g' value . ESR spectra of organic free radicals , McConnel relation , applications of ESR.

Principles of Mossbauer spectroscopy: basic principles, achirality of nucleus, Isomer shifts. Quadrupole and Nuclear Zeeman splittings. Applications in structure determination.

Text Books (Molecular Spectroscopy)

1. C. N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy, Springer, 4th edn, 2004.
2. J. M. Hollas, Modern Spectroscopy, Wiley, 4th edn, 2003.

Reference Books

1. Electron Paramagnetic Resonance, Elementary Theory and Practical Applications, Weil, John A, J. R. Bolton, and Wertz, J. E, Wiley-Interscience, New York, (1994).
2. Basic One- and Two-Dimensional NMR Spectroscopy, H. Friebolin, VCH, 1991.
3. Bunker & Jensen, Molecular Symmetry & Spectroscopy, 1998.
4. Bernath, Spectra of Atoms and Molecules, 1995.

MCYC150 INORGANIC CHEMISTRY –I LABORATORY (0-0-6) (3 credits)

I. Semi micro qualitative analysis of inorganic mixtures containing anions, common cations, less familiar element (W, Mo, Ce, Th, Zr, V and U), insoluble (sulphate, oxides, halide).

II. Preparation and quantitative analysis of complexes

- Cis-potassium diaquabis(oxalate)chromate(III) complex [analysis of oxalate and chromium]
- Hexamminecobalt(III)chloride [analysis of cobalt]
- hexamminenickel(II)chloride [analysis of nickel]
- Preparation of pentamminechloro cobalt(III)chloride.
- Chrome alum
- Copper(I) chloride
- Tris(thiourea) copper(I) complex
- Potassium tris-(oxalato)aluminate(III)
- Hexaaminecobalt(III) chloride
- Tetraaminecopper(II) sulphate.

III. Volumetric analysis

- Volumetric estimation of Ca and Mg in Dolomite solution.
- Volumetric estimation of Cu in Cu and Ni (German Silver).
- Volumetric estimation of Fe in Cu and Fe solution.
- Volumetric estimation of Zn in Cu and Zn solution.
- Volumetric estimation of Ni in Ni and Zn solution.

Selected Text/Reference Books:

1. G., Svehla, Vogel's Qualitative Inorganic Analysis, 6th Edn., Orient Longman New Delhi, l987.
2. V.V. Ramanujam, Inorganic Semi-micro Qualitative Analysis, 3rd Edn., National Publishing Company, Madras, l990.
3. J. Bassett, G. H. Jeffery and J. Mendham, and R. C. Denny,Vogel's text book of Quantitative Chemical Analysis, 5th Edition, Longman Scientific and Technical (1999).
4. Hand-outs prepared for the laboratory experiments: collections from various literature sources
5. Elias, A. J., A Collection of Interesting General Chemistry Experiments, Universities Press, (India) Pvt. Ltd., 2002.
6. Roesky, H. W.; Möckel, K., Chemical Curiosities: spectacular experiments and inspired quotes, VCH, 1996.

1ST SEMESTER/ MCYC151 ORGANIC CHEMISTRY PRACTICAL (0-0-6) (3 Credits)

Qualitative Analysis

i. Identification of organic compounds, separation, purification and identification of compounds of binary mixture using TLC and column chromatography. Interpretation of IR spectra for functional group identification.
ii. Isolation of active natural products (caffeine, lycopene, etc.) from natural sources.
iii. Preparation of paracetamol, aspirin, and some dyes and indicators.
iv. Application of steam distillation in isolation of essential oil (clove) and perfume (rose).
v. Preparation of o-iodobenzoic acid from anthranilic acid, furoic acid from furfural.
vi. Thiamine catalysed benzoin condensation
vii. P reparation of benzil from benzoin.
viii. Estimation of phenol, aniline, ascorbic Acid.
ix. Estimation of glucose by Fehling's method & Bertrand's method.

Structure Drawing of various organic building blocks using chemdraw softwares

Text Books

1. Experiments and Techniques in Organic Chemistry, D. J. Pasto, C. R. Johnson & M. J. Miller, Printice Hall, 1992.

2. Systematic Qualitative Organic Analysis, H. Middleton, E. Arnold (publisher)

3. Hand Book of Organic Analysis, Qualitative & Quantitative, M. T. Clarke, E. Arnold (publisher)

4. A. I. Vogel, 'Text book of Practical Organic Chemistry',5th Edn. ELBS, London, l989.
5. Macroscale and Microscale Organic Experiments, K. L. Williamson, D. C. Heath.