



**JAI HIND COLLEGE
BASANTSING INSTITUTE OF SCIENCE
&
J. T. LALVANI COLLEGE OF COMMERCE
(AUTONOMOUS)**

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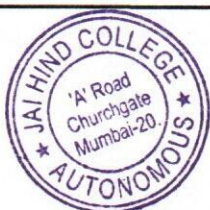
**Affiliated to
University of Mumbai**

Program: M.Sc. Chemistry
(Inorganic)

Course: Organometallics and Inorganic Polymers

Semester IV

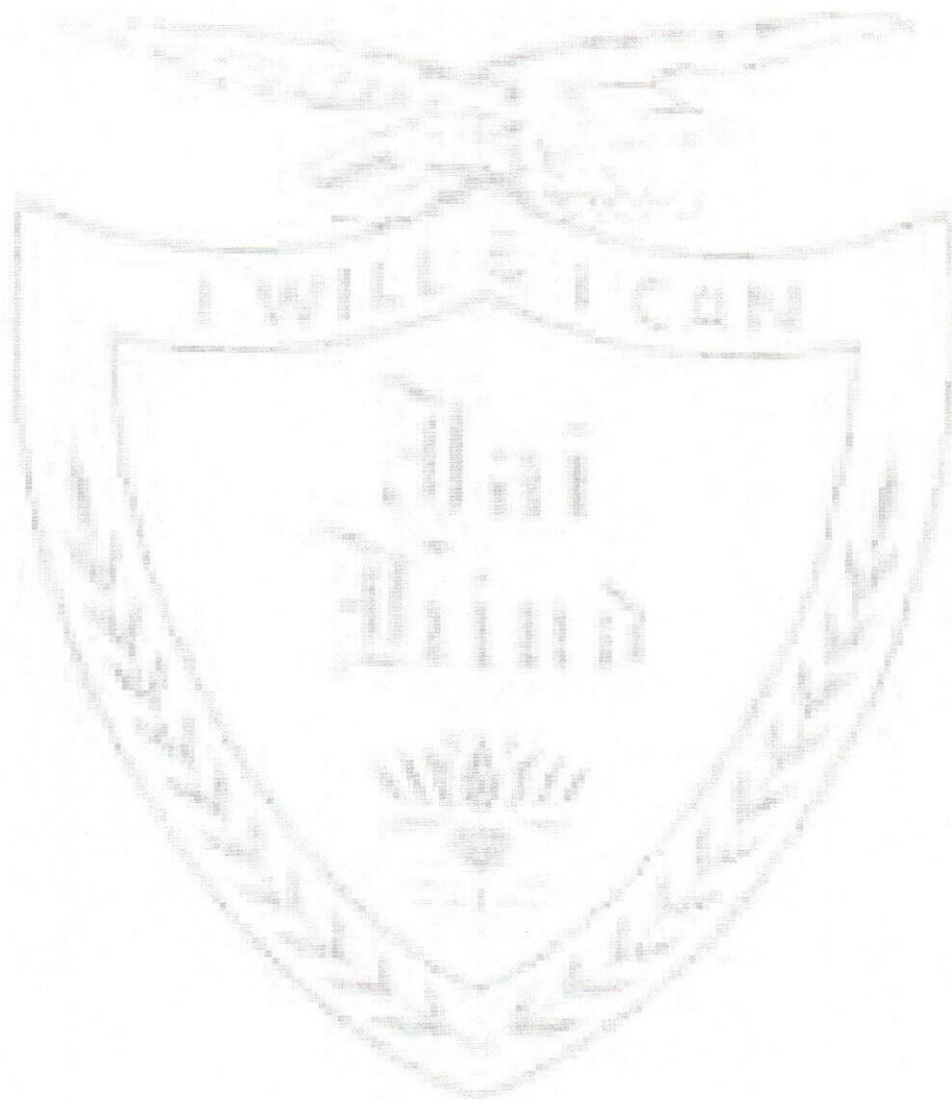
**Credit Based Semester and Grading System (CBSGS) with effect from
the academic year 2022-23**




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M.Sc. Organometallics and Inorganic Polymers Syllabus

Semester IV			
Course Code	Course Title	Credits	Lectures/Week
PSCHE2401	Organometallics and Inorganic Polymers	04	04




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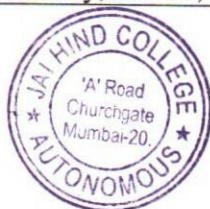
Semester IV – Theory

Course: PSCHE2401	Organometallics and Inorganic Polymers (Credits: 04 Lectures/Week: 04)	
Chemistry of Organometallic compounds and its applications in synthetic organic chemistry, inorganic polymers of silicon, phosphorus and polyionic compounds, reactivity of chemical species.		
Objectives: <ol style="list-style-type: none"> 1. To explain the metal-metal bonding in inorganic clusters and cage compounds. 2. To explain the application of organic compounds in coupling reactions. 3. To introduce the preparation, properties and application inorganic polymers. 4. To understand the concept of different Hard-Soft Acids & Bases. Outcomes: <ol style="list-style-type: none"> 1. To describe the bonding in boranes, heteroboranes, carboranes and cluster compounds. 2. To identify the application of organic compounds in coupling reactions. 3. To discuss the different preparative methods, various properties and applications of inorganic polymers. 4. To define the concept of Hard-Soft Acids & Bases. 		
Unit I	Organometallic Chemistry <ol style="list-style-type: none"> 1.1 Metal-metal bonding and Metal Clusters: <ol style="list-style-type: none"> i. Dinuclear cluster ii. Multinuclear carbonyl cluster: LNCC & HNCC, Capping rule (limitations & exceptions) iii. Mingo's rule 1.2 Structures of clusters: Electron count, Wade's Rule and Isolobal analogy 1.3 Oxidative addition & elimination reaction: Concerted additions, SN2 reactions, radical mechanisms, ionic mechanisms, reductive elimination, σ-Bond metathesis, oxidative coupling and reductive cleavage. 1.4 Inorganic Cluster and Cage compounds: introduction, bonding in boranes, heteroboranes, carboranes and cluster compounds 	15L
Unit II	Applications of Organometallic Compounds <ol style="list-style-type: none"> 2.1 Homogenous catalysts in organic reactions: <ol style="list-style-type: none"> i. Hydrosilation ii. Hydroboration 	15L




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	<ul style="list-style-type: none"> iii. Water gas Shifts Reaction iv. Wacker process (Oxidation of alkenes) v. Alcohol carbonylation <p>2.2 Olefin metathesis reactions</p> <p>2.3 Coupling reactions:</p> <ul style="list-style-type: none"> i. Heck reaction ii. Suzuki reaction iii. Sonogashira coupling iv. Stille coupling v. Kumada coupling vi. Negishi coupling vii. Hiyama Coupling viii. Buchwald-Hartwig C-N Coupling 	
Unit III	<p>Inorganic Polymers</p> <p>3.1 Silicon based: Silicates, polysilicates and aluminosilicates (Preparation, properties and applications)</p> <p>3.2 Phosphorus based: Phosphazenes, phosphazene polymers (Preparation, properties and applications)</p> <p>3.3 Polyionic species: Polyanionic and polycationic compounds</p>	15L
Unit IV	<p>Reactivity of Chemical Species II</p> <p>4.1 Pourbaix Diagrams</p> <p>4.2 Properties: Amphoteric behavior, periodic trends in amphoteric properties of p-block and d-block elements.</p> <p>4.3 Oxoions: Oxoanions and oxocations</p> <p>4.4 Hard-Soft Acids & Bases: Measure of hardness and softness of acids and bases, Drago-Wayland equations</p> <p>4.5 Applications of acid-base Chemistry: Super acids and super bases, heterogeneous acid-base reactions</p>	15L
<p>Standard References:</p> <ol style="list-style-type: none"> 1. Gary Wulfsberg, Inorganic Chemistry ; Viva Books PA Ltd., New Delhi; 2002. 2. F.A. Cotton and Wilkinson, Advanced Inorganic Chemistry, 3rd edition. 3. D.F. Shriver, P.W. Atkins and C.H. Langford, Inorganic Chemistry, 3rd edition Oxford University Press, 1999. 4. J.D. Lee, Concise Inorganic Chemistry, 5th ed., Blackwell Science Ltd., 		





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5. R.H. Crabtree, The Organometallic Chemistry of the Transition Metals, Wiley-Interscience, New York, 1988.
 6. G.W.Parshall and S.D.Ittel, Homogeneous Catalysis, 2nd edition, John Wiley & sons, Inc., New York, 1992.
 7. Gary O. Spessard and Gary L.Miessler, Organometallic Chemistry, Prentice-Hall, (1997).
 8. B.D.Gupta & Anil Elias, Basics in Organometallic chemistry
 9. . R.C.Mehrotra and A.Singh, Organometallic Chemistry-A Unified Approach, 2nd ed., New Age International Pvt.Ltd., 2000.
 10. B.Douglas, D.H. McDaniel and J.J.Alexander, Concepts and Models of Inorganic Chemistry, 2nd edition, John Wiley & Sons, 1983.
 11. James E.Huheey, Inorganic Chemistry-Principles of structure and reactivity, edn Harper & Row Publishers (1972).
 12. . F. A. Cotton, G. Wilkinson, C. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th ed., John Wiley, New York, 1999.

Evaluation Scheme

- **Continuous Assessment (CA) – 40 Marks**
 - Knowledge and Application based: Objective test of 20 Marks
 - Skill based (20 marks): Learner will be assessed on relevant skills pertaining to the course content of a particular paper which could involve but not limited to
 - Oral Presentations on relevant topics
 - Review writing/Worksheets etc.
- **Semester End Examination (SEE)- 60 Marks**




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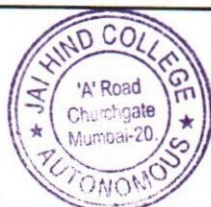
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Program: M.Sc. Chemistry
(Inorganic)

Course: Practical Coursework III

Semester IV

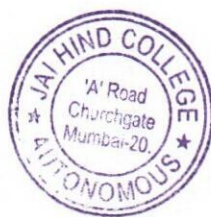
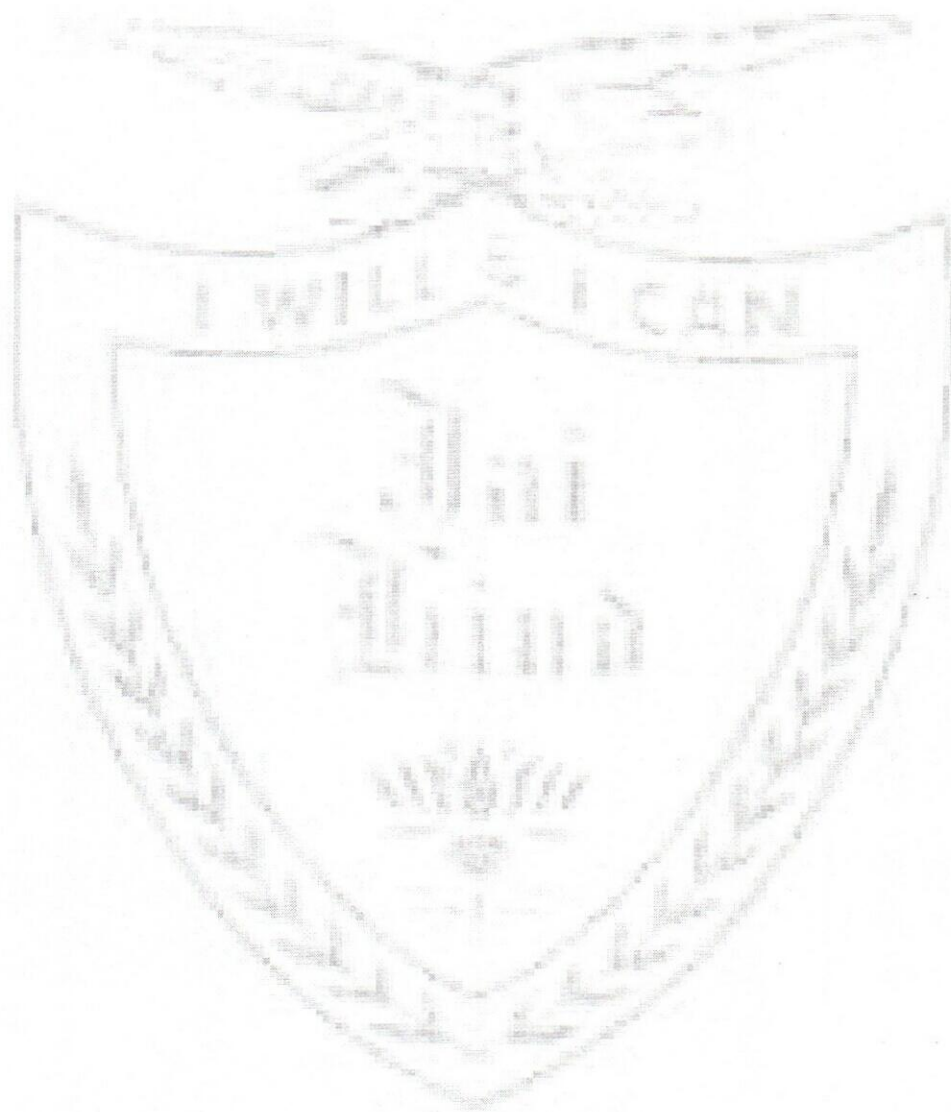
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M.Sc. Practical Coursework III Syllabus

Semester IV			
Course Code	Course Title	Credits	Lectures/Week
PSCHEP2401	Practical Coursework III	02	02




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Semester IV – Practical

Course: PSCHEP2401	Practical Coursework III (Credits: 02, Practical/Week: 02)
	Objectives: To solve problems in chemistry through experiments.
	Outcomes: Learner will be able to design experiments and will gain experimental skills to solve problems in chemistry
PSCHEP2401: Practical Coursework III	
<ol style="list-style-type: none">1. Determination of the transport number of Silver(I) ions by Hittorf's method.2. To study the order of the reaction between bromate and bromide.3. To determine the van't Hoff's factor by cryoscopic method.4. To determine K_1 and K_2 of a dibasic acid by titration with a base by pH metry.5. To determine the composition of a mixture of HCl, KCl and NH_4Cl by titration with NaOH and AgNO_3.6. To determine the liquid junction potential with a concentration cell with and without transference.	
REFERENCES:	
<ol style="list-style-type: none">1. Jeffery G.H., Bassett J., Mendham J., Denney R.C., Vogel's Textbook of Quantitative Chemical Analysis, 5th Edition, Longman Scientific & Technical John Wiley & Sons Inc., New York, 19892. Woolins J.D., Inorganic Experiments, VCH, Weinheim, 19943. Palmer W.G., Experimental Inorganic Chemistry, CUP Archive 19544. Raj G., Advanced Practical Inorganic Chemistry, Krishna Prakashan Media (P) Ltd, 20135. Daniel F. & Others, Experimental Physical Chemistry, 1965, Kogakasha Co Ltd. Tokyo6. Athawale V.D., Mathur P., Experimental Physical Chemistry, New Age International Publishers, 2017.7. Vishwanathan B., Raghavan P.S., Practical Physical Chemistry, Viva Books Private Limited, 20058. James A.M., Prichard F.E., Practical Physical Chemistry, 3rd Edition, Longman, 19749. Lewitt B.P., Findlay's Practical Physical Chemistry, 9th Edition, 197310. Brennan C.D., Tipper C.F.H., A Laboratory Manual of Experiments in Physical Chemistry, McGraw Hill 196711. Daniel F. & Others, Experimental Physical Chemistry, 1965, Kogakasha Co Ltd. Tokyo	

Evaluation Scheme

- Semester End Examination (SEE)- 50 Marks



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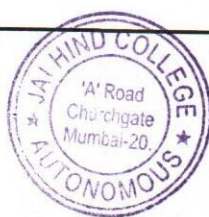
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Program: M.Sc. Chemistry
(Inorganic)

Course: Solid State Chemistry

Semester IV

**Credit Based Semester and Grading System (CBSGS) with effect from
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M.Sc. Solid State Chemistry Syllabus

Semester IV			
Course Code	Course Title	Credits	Lectures/Week
PSCHE2402	Solid State Chemistry	04	04



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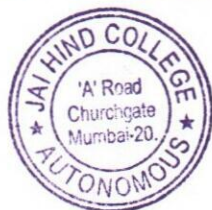
Semester IV – Theory

Course: PSCHE2402	Solid State Chemistry (Credits: 04 Lectures/Week: 04)	
	Solid state- structure, properties and synthesis; defects and non-stoichiometry, electrical, magnetic, thermal and optical properties of solids	
	Objectives: <ol style="list-style-type: none"> 1. To understand the Structure, properties and Synthesis of solids. 2. To understand the crystal defects and non-stoichiometry. 3. To introduce the Electrical and Magnetic Properties of solids. 4. To summarise the thermal and optical properties of solids. Outcomes: <ol style="list-style-type: none"> 1. To distinguish between different structure of solids and various method to synthesize it. 2. To identify different type of defects and its applications. 3. To describe the electrical, magnetic, thermal and optical properties of solid. 	
Unit I	Structure, properties and Synthesis of solids <ol style="list-style-type: none"> 1.1 Simple structures: <ol style="list-style-type: none"> (i) AB type compounds (PbO & CuO) (ii) AB₂type (β cristobalite, CaC₂ and Cs₂O) (iii) AB₃type (ReO₃, Li₃N) (iv) ABO₃type, relation between ReO₃ and perovskite BaTiO₃, its polymorphic forms, oxide bronzes, ilmenite structure (v) AB₂O₄type, normal, inverse, and random spinel structures 1.2 Linked Polyhedra <ol style="list-style-type: none"> (i) Corner sharing: tetrahedral structure (silicates) and octahedral structure (ReO₃) and rotation of ReO₃ resulting in VF₃, RhF₃ and calcite type structures (ii) Edge sharing: tetrahedral structures (SiS₂) and octahedral structures (BiI₃ and AlCl₃), pyrochlores, octahedral tunnel structures and lamellar structures 1.3 Methods of synthesis: Chemical method, high pressure method, arc technique and Skull method (with examples). 1.4 Single crystal growth: Crystal growth from melt- Bridgman <ol style="list-style-type: none"> (i) Crystal growth from melt: Bridgman and Stockbargar, Czochralski and Vernuil methods (ii) Crystal growth from liquid solutions: Flux growth and temperature gradient methods (iii) Crystal growth from vapour phase: epitaxial growth methods. 	15L




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Unit II	Crystal defects and non-stoichiometry 2.1 Point defects: Point defects in metals and ionic Crystals – Frenkel defect and Schottky defect;thermodynamic formation of these defects (mathematical derivation to find defect concentration); defects in non-stoichiometric compounds, color centers 2.2 Line defects: Edge and Screw Dislocations. Mechanical Properties and Reactivity of Solids 2.3 Surface defects: Grain Boundary and Stacking Fault. Dislocation and Grain Boundaries, Vacancies and Interstitial Space in Non-Stoichiometric Crystals, Defect Clusters, Interchangeable Atoms and Extended Atom Defects	15L
Unit III	Electrical and Magnetic Properties of Solids 3.1 Electrical properties of solids: Conductivity of solid electrolytes, fast ion conductors, mechanism of conductivity, hopping conduction, Thomson and Seebeck Effects; Thermocouples and their applications, Hall effect, Dielectric, ferroelectric, piezoelectric and pyroelectric materials and their inter-relationships and applications 3.2 Magnetic properties: Behaviour of substance in magnetic field, mechanism of ferromagnetic and antiferromagnetic ordering, Hysteresis, Hard and soft magnets; Structures and magnetic Properties of Metals and Alloys; Transition metal Oxides; Spinels; garnets, Ilmenites;Perovskite and Magneto plumbites, Application in transformer cores, information storage, magnetic bubble memory devices and as permanent magnets	15L
Unit IV	Thermal and Optical Properties of Solids 4.1 Thermal properties: Introduction, heat capacity and its temperature dependence; thermal expansion of metals; ceramics and polymers and thermal stresses 4.2 Optical properties: Color Centres and Birefringence; Luminescent and Phosphor Materials; Coordinate Model; Phosphor Model; Anti Stokes Phosphor	15L
Standard References: 1. L. E. Smart and E. A. Moore, Solid State Chemistry-An introduction, 3rd edition, Taylor and Francis, 2005. 2. A.R.West, Solid State Chemistry and Its Applications, John Wiley & sons, 1987. 3. C.N.R. Rao and J.Gopalkrishnan New Directions in Solid State Chemistry, 2nd		



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 9. H.V.Keer, Principles of the Solid state, Wiley Eastern Ltd., 1993. Gary L.Miessler and Donald A.Tarr, Inorganic Chemistry, 3rd edition , Pearson Education, Inc., 2004.
 10. D.K.Chakraborty, Solid State Chemistry, New Age International Publishers, 1996.
 11. A. Earnshaw, Introduction to Magnetochemistry, Acad. Press,N.Y. (1966)

Evaluation Scheme

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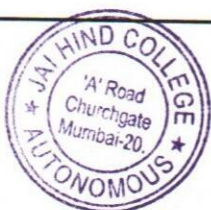
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Program: M.Sc. Chemistry
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Course: Practical Coursework IV
Semester IV

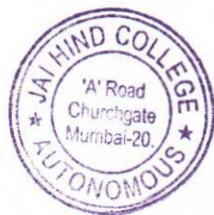
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M.Sc. Practical Coursework IV Syllabus

Semester IV			
Course Code	Course Title	Credits	Lectures/Week
PSCHEP2402	Practical Coursework IV	02	02




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Semester IV – Practical

Course: PSCHEP2402	Practical Coursework IV (Credits: 02, Practical/Week: 02)
	Objectives: To evaluate commercial samples, ores and alloys for their percentage assay.
	Outcomes: Learner will be introduced to quality control procedures, errors in measurement and comparison against standards.
	PSCHEP2402: Practical Coursework IV <ol style="list-style-type: none">Analysis of commercial sample of electrical powder for Na⁺ content by flame photometerAnalysis of commercial sample of sea water for percentage salinity by Volhard's method.Analysis of commercial sample of Fasting salt for chloride content by conductometricallyDetermination of Stability constant of [Ag(en)]⁺ by potentiometryAnalysis of Galena ore for Pb content by gravimetry & Fe by colorimetryAnalysis of Brass alloy for Cu content by iodometrically and Zn complexometrically
	REFERENCES: <ol style="list-style-type: none">Jeffery G.H., Bassett J., Mendham J., Denney R.C., Vogel's Textbook of Quantitative Chemical Analysis, 5th Edition, Longman Scientific & Technical John Wiley & Sons Inc., New York, 1989Woolins J.D., Inorganic Experiments, VCH, Weinheim, 1994Palmer W.G., Experimental Inorganic Chemistry, CUP Archive 1954Raj G., Advanced Practical Inorganic Chemistry, Krishna Prakashan Media (P) Ltd, 2013Daniel F. & Others, Experimental Physical Chemistry, 1965, Kogakasha Co Ltd. TokyoAthawale V.D., Mathur P., Experimental Physical Chemistry, New Age International Publishers, 2017.Vishwanathan B., Raghavan P.S., Practical Physical Chemistry, Viva Books Private Limited, 2005James A.M., Prichard F.E., Practical Physical Chemistry, 3rd Edition, Longman, 1974Lewitt B.P., Findlay's Practical Physical Chemistry, 9th Edition, 1973Brennan C.D., Tipper C.F.H., A Laboratory Manual of Experiments in Physical Chemistry, McGraw Hill 1967Daniel F. & Others, Experimental Physical Chemistry, 1965, Kogakasha Co Ltd. Tokyo




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Evaluation Scheme

- Semester End Examination (SEE)- 50 Marks




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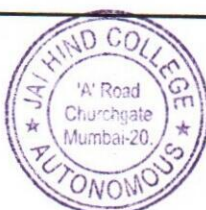
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Program: M.Sc. Chemistry
(Inorganic)

Course: Photochemistry and Advanced Spectroscopy

Semester IV

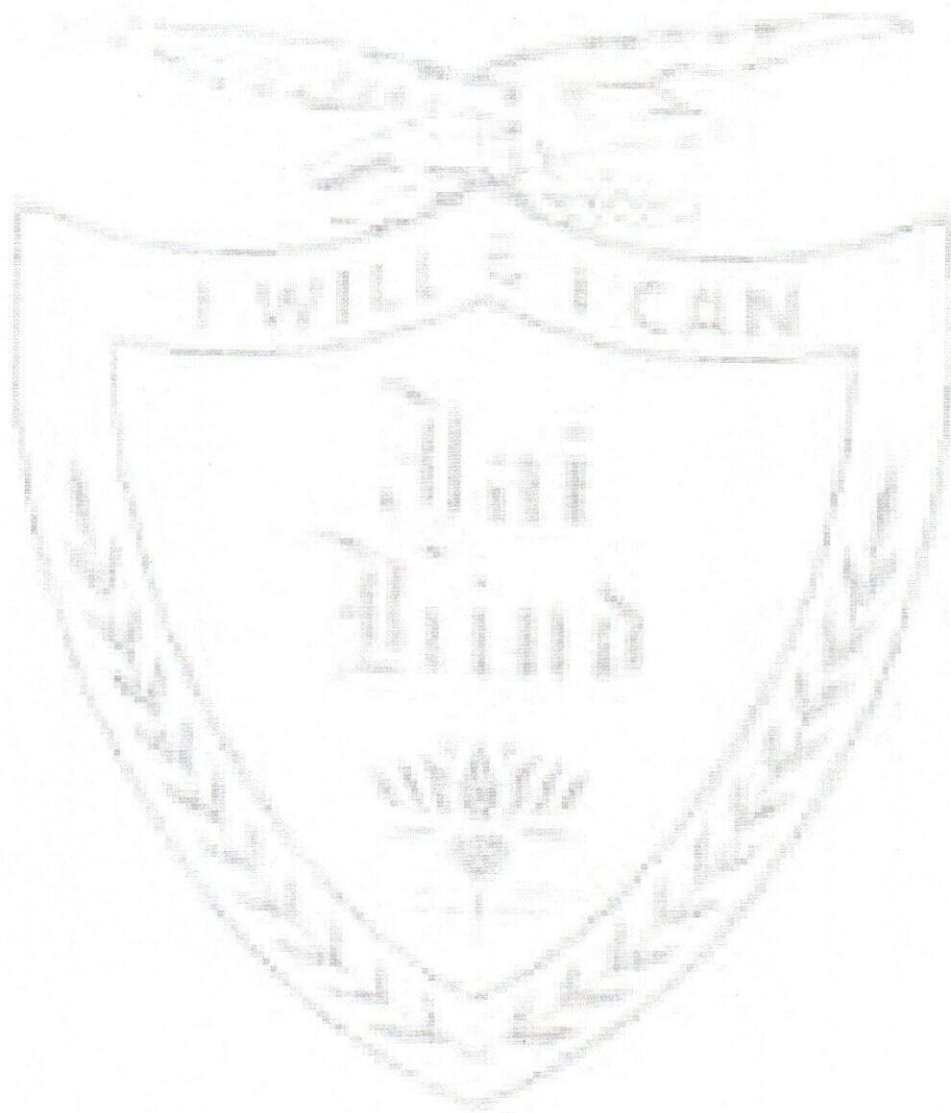
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M.Sc. Photochemistry and Advanced Spectroscopy Syllabus

Semester IV			
Course Code	Course Title	Credits	Lectures/Week
PSCHE2403	Photochemistry and Advanced Spectroscopy	04	04




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Semester IV – Theory

Course: PSCHE2403	Photochemistry and Advanced Spectroscopy (Credits:04 Lectures/Week:04)	
	Photochemistry and photocatalysis, fluorescence phenomenon and its applications, advanced techniques in NMR spectroscopy & mass spectrometry	
	Objectives: <ol style="list-style-type: none"> 1. To introduce the concept of Photochemistry & Photocatalysis. 2. To understand the principal and application of fluorescence phenomena. 3. To describe the principal, instrumentation and applications of advanced Spectroscopic Techniques-I& II. Outcomes: <ol style="list-style-type: none"> 1. To apply the principles of Photochemistry & Photocatalysis in water splitting, CO₂ reductions etc. 2. To describe the phenomena and mechanism of fluorescence quenching. 3. To elucidate the structure of molecules applying advanced Spectroscopic Techniques-I & II. 	
Unit I	Photochemistry & Photocatalysis 1.1 Photochemistry [8L] <ol style="list-style-type: none"> 1.1 General Introduction: Laws of photochemistry, selection rules for transitions, shapes of absorption bands and Frank Condon Principle. 1.2 Properties of excited state: Environmental effect on absorption and emission spectra, solvatochromic shifts, properties of excited state- dipole moment, acidity constant, redox potential. 1.3 Photophysical pathways: types of photophysical pathways, types of radiationless transitions, fluorescence emission, triplet state and phosphorescence, delayed fluorescence: e-type and p-type. 1.2 Photocatalysis [7L] <ol style="list-style-type: none"> 1.4 Photocatalytic activity: Photocatalytic reactions, mechanism, influence of different parameters on catalytic activity. 1.5 Types of photocatalysts: SMOs (TiO₂, ZnO), metal chalcogenides (MoS₂, WS₂), quantum dots (C, S), mesoporous materials for photocatalysis and their synthesis (one each) 1.6 Application of photocatalysis: photodegradation of organic pollutants, CO₂ photoreduction, water splitting. 	15L




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Unit II	<p>Applications of Fluorescence Phenomena</p> <p>2.1. Introduction & Fluorescence Characteristics: Fluorescence phenomenon, Characteristics of fluorescence-mirror image rule, exceptions, Kasha's Rule; Stokes shift, fluorescence lifetimes and quantum yields, steady state fluorescence and fluorescence anisotropy [2L]</p> <p>2.2. Structural effects on Fluorescence emission: π-electron system, substituted aromatic hydrocarbons- internal heavy atom effect, EDG, EWG, Sulfonates, heterocyclic compounds- Nitrogen heterocycles, coumarins, BODIPY; Luminescence of nanostructures- carbon nanostructures, quantum dots. [2L]</p> <p>2.3. Fluorescence quenching: mechanism of quenching- static and dynamic; derivation of Stern-Volmer equations for static and collisional quenching, quenching by added substances-charge transfer mechanism (CT) and energy transfer mechanism (RET) [3L]</p> <p>2.4. Instrumentation and sensing: instrumentation of a steady state spectrofluorophotometer, modes of measurement- fixed excitation wavelength, fixed emission wavelength, fixed excitation and emission wavelength, variable excitation and emission wavelengths- 3D spectrum, synchronous spectrum; analytical terms associated with sensing- sensitivity, selectivity & ICH guidelines- LOD, LOL, dynamic range [4L]</p> <p>2.5. Applications of Fluorescence: Sensing modes and mechanisms, Photoinduced Electron Transfer (PET), Photoinduced Charge Transfer (PCT); design of sensor; miscellaneous applications of fluorescence [4L]</p>	15L
Unit III	<p>Advanced Spectroscopic Techniques-I</p> <p>3.1 Basic Concepts in NMR: Nuclear spin states, magnetic moments, absorption of energy, mechanism of absorption, population densities of nuclear spin states, chemical shift and shielding, NMR spectrometer- CW v/s FT NMR [4L]</p> <p>3.2 Spin-spin coupling: spin-spin splitting (n+1) rule, origin of spin-spin splitting and Pascal's triangle, coupling constant J, mechanism of coupling, Karplus relationship, long range coupling, magnetic equivalence, first order splitting and complex multiplets- more than one value of J, second order spectra and Pople spin notations; second order effects and field strength of NMR. [5L]</p> <p>3.3 ^{13}C & Heteronuclear NMR: ^{13}C nucleus, chemical shifts, proton coupled and decoupled ^{13}C NMR, NOE & cross polarization, molecular relaxation processes & integration of</p>	15L




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	<p>spectra, Off-resonance decoupling, solvents used in NMR; ^{19}F, ^{31}P, ^{11}B NMR; heteronuclear coupling of ^{13}C with fluorine and phosphorus. [4L]</p> <p>3.4 Other topics in 1D NMR: proton exchange, dynamic NMR, quadrupole broadening of NH protons [2L]</p>	
Unit IV	<p>Advanced Spectroscopic Techniques II:</p> <p>4.1 Pulsed techniques in NMR: FT-NMR, Attached Proton Test (APT), INEPT & DEPT [4L]</p> <p>4.2 2D NMR techniques: Homonuclear 2D NMR- COSY, NOESY; Heteronuclear 2D NMR- HETCOR, HSQC, HMQC, HMBC [4L]</p> <p>4.3 Mass spectrometer: Overview, block diagram & sample introduction [1L]</p> <p>4.4 Ionization methods: Electron ionization (EI); Chemical ionization (CI); Desorption ionization methods (SIMS, FAB, MALDI); Electron spray ionization (ESI) [3L]</p> <p>4.5 Mass analyzers: Magnetic sector, double focusing, Quadrupole, TOF; detection and quantitation; determination of molecular weight & molecular formulae [3L]</p> <p>Spectral problems: Application of NMR & Mass Spectrometry in structure elucidation.</p>	15L
<p>Standard References:</p> <p>Unit I</p> <ol style="list-style-type: none"> 1. Rohatgi-Mukherjee, K. K. (1992). Fundamentals of photochemistry. New Delhi: Wiley Eastern Ltd, 2. Photocatalysis- Principles and Applications, Rakshit Ameta, Suresh C.Ameta, CRC Press, Taylor & Francis group, Boca Raton, London, New York, 2017. 3. Zhang, J., Tian, B., Wang, L., Xing, M., Lei, J. - Photocatalysis_ Fundamentals, Materials and Applications-SPRINGER VERLAG, SINGAPORE (2018) <p>Unit II</p> <ol style="list-style-type: none"> 4. Lakowicz, J. R. (2006). Principles of fluorescence spectroscopy. New York: Springer. 5. Valeur, B. (2002). Molecular fluorescence: Principles and applications. Weinheim: Wiley-VCH. <p>Unit III & IV</p> <ol style="list-style-type: none"> 6. Pavia, D. L., Lampman, G. M., & Kriz, G. S. (1979). Introduction to spectroscopy: A guide for students of organic chemistry. Philadelphia: W.B. Saunders Co 7. Field, L. D., Li, H. L., & Magill, A. M. (2015). Organic structures from 2D NMR spectra. 		



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Additional References:

8. Spectroscopy of Organic compounds, P.S. Kalsi, New Age International Pub. Ltd. And Wiley Eastern Ltd., Second edition, 1995.
9. Applications of Absorption Spectroscopy of Organic compounds, J. R. Dyer, Prentice Hall of India, 1987.
10. Spectrometric Identification of Organic compounds, R.M. Silverstein and others, John Wiley and Sons Inc., 5th ed., 1991
11. Absorption spectroscopy of organic Molecules, V.M. Parikh, 1974.
12. Spectroscopic methods in organic chemistry, Williams and Fleming, Tata McGraw Hill, 4th ed, 1989.
13. Organic spectroscopy, William Kemp, ELBS, 3rd ed., 1987.

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BASANTSING INSTITUTE OF SCIENCE
&
J.T.LALVANI COLLEGE OF COMMERCE
(AUTONOMOUS)**

"A" Road, Churchgate, Mumbai - 400 020, India.


**Affiliated to
University of Mumbai**

Program: M.Sc. Chemistry
(Inorganic)

Course: Spectral Interpretation
Semester IV

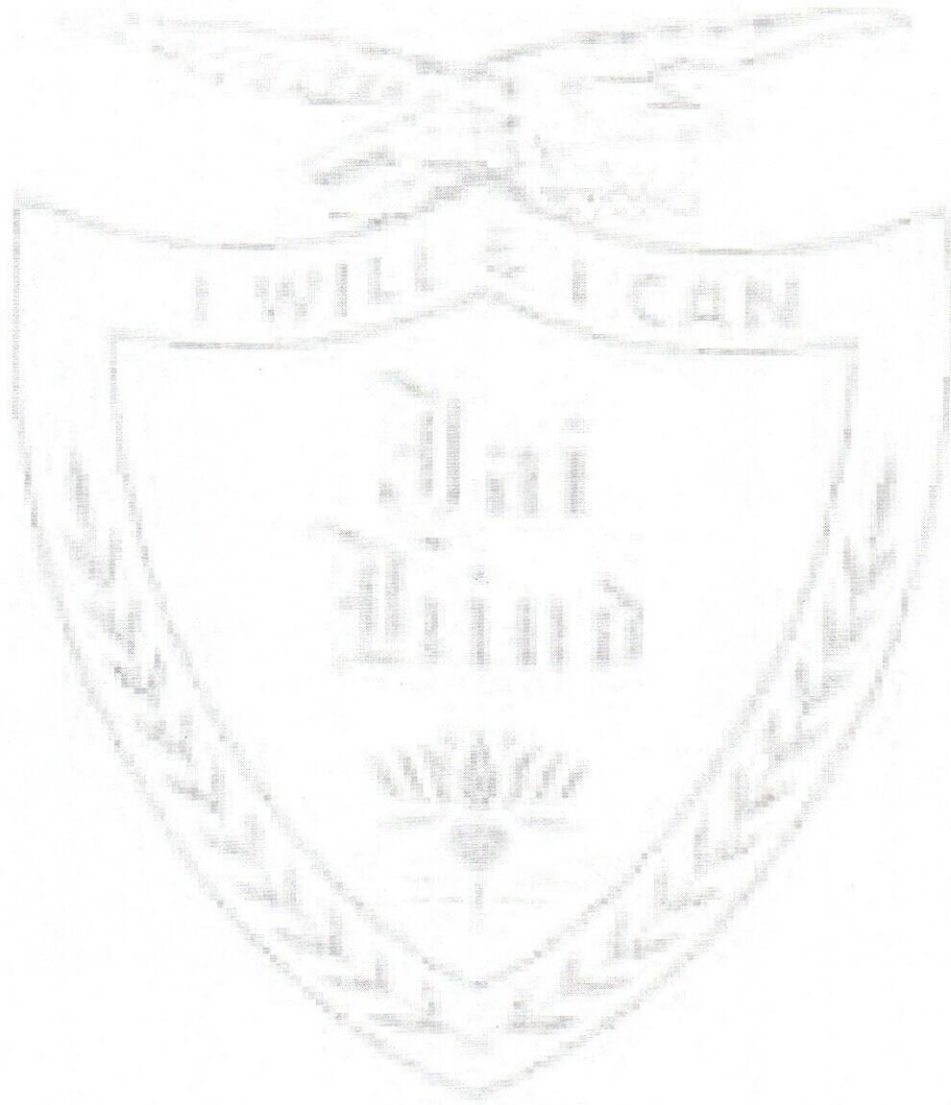
**Credit Based Semester and Grading System (CBSGS) with effect from
the academic year 2022-23**




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M.Sc. Spectral Interpretation Syllabus

Semester IV			
Course Code	Course Title	Credits	Lectures/Week
PSCHEP2403	Spectral Interpretation	02	02




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Semester IV – Practical

Course: PSCHEP2403	Spectral Interpretation (Credits: 02, Practical/Week: 02)
	Objectives: To elucidate structural information about molecules from their spectral data.
	Outcomes: Learner will be able to interpret of UV/IR/NMR/Mass/XRD spectra and its analysis.
PSCHEP2403: Spectral Interpretation	
Interpretation of UV/IR/NMR/Mass/XRD spectra and its analysis.	
REFERENCES:	
1. Jeffery G.H., Bassett J., Mendham J., Denney R.C., Vogel's Textbook of Quantitative Chemical Analysis, 5 th Edition, Longman Scientific & Technical John Wiley & Sons Inc., New York, 1989	

Evaluation Scheme

- Semester End Examination (SEE)- 50 Marks




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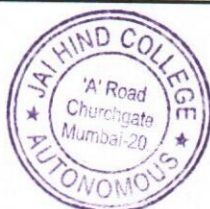
Program: M.Sc. Chemistry

(Inorganic)

Course: Materials, Devices and Computational Chemistry

Semester IV

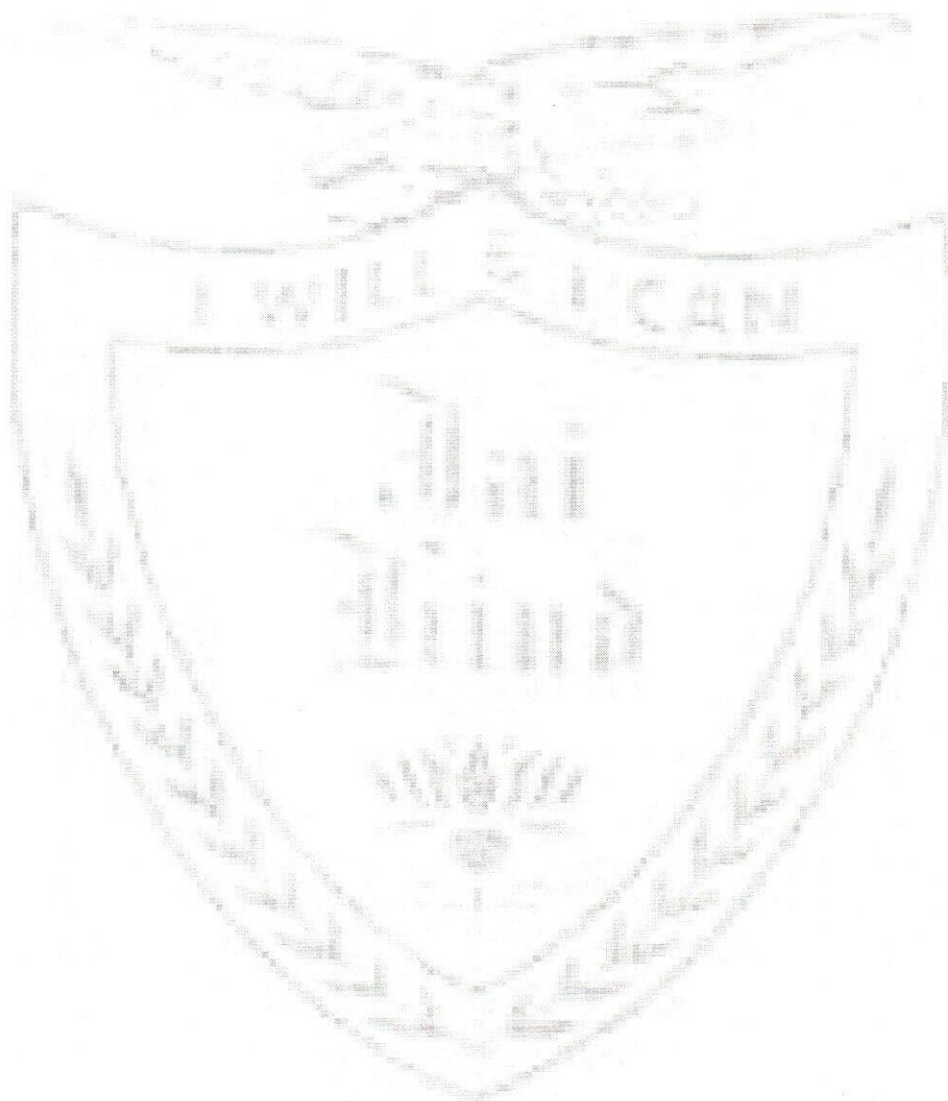
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M.Sc. Materials, Devices and Computational Chemistry Syllabus

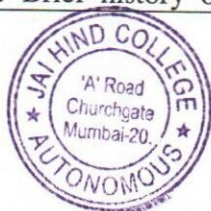
Semester IV			
Course Code	Course Title	Credits	Lectures/Week
PSCHE2404	Materials, Devices and Computational Chemistry	04	04




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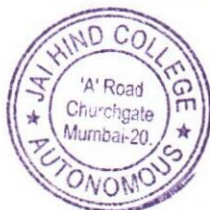
Semester IV – Theory

Course: PSCHE2404	Materials, Devices and Computational Chemistry (Credits:04 Lectures/Week:04)	
	Solar photovoltaics, batteries and supercapacitors, organic electronic and photonic materials, Intellectual Property Rights & Cheminformatics	
	Objectives: <ol style="list-style-type: none"> 1. To describe different photovoltaic cells and its applications in batteries and supercapacitors. 2. To introduce the concept of organic semiconductors, optoelectronic devices. 3. To introduce the of Intellectual Property Rights & Cheminformatics. Outcomes: <ol style="list-style-type: none"> 1. To identify different type photovoltaic cells and its applications in batteries and supercapacitors. 2. To explain the working of organic semiconductors, optoelectronic devices. 3. To describe Intellectual Property Rights & Cheminformatics. 	
Unit I	Energy Conversion and Storage Devices <ol style="list-style-type: none"> 1. Solar Photovoltaics: P-n junction, light generating current, I-V equation, solar characteristics, effects of various parameters on efficiency, losses in solar cells, Solar cell design, Antireflective coating (ARC), solar simulator, Quantum efficiency. [5L] 2. Sensitized and polymer photovoltaics: DSSC, Quantum dot sensitised solar cells, Perovskite sensitised solar cells, Planar and bulk heterojunction polymer solar cells, Exciton generation and dissociation, Advantages, disadvantages, and types of materials. [4L] 3. Batteries and Supercapacitors: Recapitulation of batteries: primary batteries, rechargeable batteries, electrochemical energy storage: laws, parameters, heat effects. Types of batteries (Lead-acid, Ni/Cd, Ni/metal hybrid), charging methods and techniques, characteristic curves, comparison of supercapacitor and batteries, Energetics, Double layer electrostatic capacitor, Pseudocapacitance, Impedance, materials for supercapacitors. [6L] 	15L
Unit II	Organic Electronic & Photonic Materials [15L] <p>3.1 Introduction: Brief history of organic electronics, organic</p>	15L




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	<p>semiconductor materials, electronic states, and transitions [2L]</p> <p>3.2 Organic semiconductors: Charge formation- By injection, By absorption, By doping; determining energy levels of charged molecules- cyclic voltammetry, photoemission spectroscopy; difference between electrical and optical gap; [5L]</p> <p>3.3 Semiconductor materials: Transport in organic materials- electrode contacts, transport regimes & magnetic field effects on transport; preparation of semiconductor materials- synthetic approaches, preparation of thin films & patterning for devices [3L]</p> <p>3.4 Optoelectronic devices: Basic processes- photon absorption, spontaneous photon emission, stimulated photon emission; Devices- OFET, OPV, OLED; molecular materials for OLEDs- hole transporting, electron transporting, emitting materials: fluorescent, phosphorescent & TADF. [5L]</p>	
Unit III	<p>Intellectual Property Rights [15L]</p> <p>3.1 Introduction to Intellectual Property: Definitions and types of IP, importance of protecting IP, economic value of IP- intangible assets and their valuation, licensing, and technology transfer laws. [2L]</p> <p>3.2 Patents: Definition, Historical perspective, Basic and associated right, WIPO, PCT system, databases in patent search- google patents, reading and writing patents [5L]</p> <p>3.3 Industrial Designs: Definition, how to obtain, features, international design registration [2L]</p> <p>3.4 Copyrights: Introduction, how to obtain, differences from Patents [2L]</p> <p>3.5 Trademarks: Introduction, how to obtain, different types of marks- collective marks, certification marks, service marks, trade names etc. [2L]</p> <p>3.6 Geographical indications: Definition, rules for registration, prevention of illegal exploitation, importance to India. [2L]</p>	15L
Unit IV	<p>Cheminformatics [15L]</p> <p>4.1 Introduction to Cheminformatics: History & evolution of cheminformatics, fundamental questions & learning, major tasks [2L]</p>	15L




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	<p>4.2 Representation of molecules: Nomenclature, different types of notations, Line notations- SMILES coding, InChi notation; Graph theory & matrix representations, input and output of chemical structures, standard structure exchange formats, structures of molfiles and sfiles, Tools- academic programs: Marvin Sketch, ACD labs; commercial tools: ChemDraw, Shrodinger, Accelrys [5L]</p> <p>4.3 Representation of chemical reactions: Reaction types, reaction center, chemical reactivity, Hendrickson's scheme [2L]</p> <p>4.4 Searching Chemical Structures: Full structure search, sub-structure search, basic ideas, similarity search, basics of computation of physical and chemical data and structure descriptors, data visualisation [2L]</p> <p>4.5 Applications: QSPR, Spectra correlations, Computer aided synthesis design, docking & computer aided drug designing [4L]</p>	
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Standard References:

Unit I

1. <https://www.pveducation.org/pvcdrom/solar-cell-operation>
2. Solar photovoltaics, Fundamentals, Technologies and Applications by Chetan Singh Solanki, PHI Learning Private Limited, Delhi-110092.
3. Dye Sensitized Solar Cells by K. Kalyansundaram, EPFL Press, A Swiss academic publisher distributed by CRC press.
4. Battery Technology Handbook by H. A. Kiehne, Marcel Dekker, Inc., New York, Basel.
5. Electrochemical Supercapacitors, Scientific fundamentals and Technological Applications by B. E. Conway, Kluwer Academic/ Plenum Publishers, New York, Boston, Dordrecht, London, Moscow.

Unit II

6. Kohler, A., & Bassler, H. (2015). *Electronic processes in organic semiconductors: An introduction*.
7. Muller, T. J. J., & Bunz, U. H. F. (2007). *Functional organic materials: Syntheses, strategies and applications*. Weinheim: Wiley-VCH.
8. Ostroverkhova, O. (2019). *Handbook of organic materials for electronic and photonic devices*.
9. Sun, S.-S., & In Dalton, L. R. (2019). *Introduction to organic electronic and optoelectronic materials and devices*.

Unit III

10. Duran, N., Fonseca, L. C., & Seabra, A. B. (2019). *Intellectual property in chemistry: A guide to applying for and obtaining a patent for graduate students and postdoctoral scholars*.

Unit IV

11. Gasteiger, J., & Engel, T. (2008). *Cheminformatics: A textbook*. Weinheim: Wiley-



VCH.

12. Andrew R. Leach & Valerie J. Gillet (2007) *An Introduction to Cheminformatics*. Springer: The Netherlands.
13. Karthikeyan, M., & Vyas, R. (2014). *Practical cheminformatics*.
14. In Engel, T., & In Gasteiger, J. (2018). *Applied cheminformatics: Achievements and future opportunities*.

Evaluation Scheme

- **Continuous Assessment (CA) – 40 Marks**
 - Knowledge and Application based: Objective test of 20 Marks
 - Skill based (20 marks): Learner will be assessed on relevant skills pertaining to the course content of a particular paper which could involve but not limited to
 - Oral Presentations on relevant topics
 - Review writing/Worksheets etc.
- **Semester End Examination (SEE)- 60 Marks**



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**Affiliated to
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Program: M.Sc. Chemistry

(Inorganic)

Course: Research Project

Semester IV

**Credit Based Semester and Grading System (CBSGS) with effect from
the academic year 2022-23**




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M.Sc. Research Project Syllabus

Semester IV			
Course Code	Course Title	Credits	Lectures/Week
PSCHEP2404	Research Project	02	02




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Semester IV – Practical

Course: PSCHEP2404	Research Project (Credits: 02, Practical/Week: 02)
	Objectives: To design a research problem and investigate it experimentally through project. Outcomes: Learners will be able to understand research workflow- literature review, identification of research problem and investigation.
PSCHEP2404: Research Project Short term research project culminating in a dissertation and presentation of the work done.	

Evaluation Scheme

- Semester End Examination (SEE)- 50 Marks




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