

M.Sc. INORGANIC CHEMISTRY

SEMESTER III

Course Code	Unit	Topics
		(Numericals and word problems wherever possible.)
PSCHI 301		1. Chemistry of Inorganic Solids
	I	1.1 Descriptive Crystal Chemistry(15 L)
		(a) Simple structures
		Structures of AB type compounds (PbO and CuO), AB₂ type (β cristobalite, CaC ₂ and Cs ₂ O), A₂B₃ type (Cr ₂ O ₃ and Bi ₂ O ₃), AB₃ (ReO ₃ , Li ₃ N), ABO₃ type, relation between ReO ₃ and perovskite BaTiO ₃ and its polymorphic forms, Oxide bronzes, ilmenite structure, AB₂O₄ type, normal, inverse, and random spinel structures.
		(b) Linked Polyhedra
		(i) Corner sharing: tetrahedral structure (Silicates) and octahedral structure (ReO ₃) and rotation of ReO ₃ resulting in VF ₃ , RhF ₃ and calcite type structures. (ii) Edge sharing: tetrahedral structures (SiS ₂) and octahedral structures (BiI ₃ and AlCl ₃). pyrochlores, octahedral tunnel structures and lamellar structures
	II	1.2 Imperfection in crystals and Non-Stoichiometry (15 Lectures)
		(a) Point defects: Point defects in metals and ionic Crystal – Frenkel defect and Schottky defect. Thermodynamics formation of these defects (mathematical derivation to find defect concentration); Defects in non-Stoichiometric compounds, colour centres.
		(b) Line defects: Edge and Screw Dislocations. Mechanical Properties and Reactivity of Solids.
		(c) 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.
	1.3 Methods of Preparations (15 Lectures)	
	(a) Methods of Synthesis: Chemical Method, High Pressure Method, Arc Technique and Skull Method (with examples).	
III		(b) Different methods for single crystal growth:
		(i) Crystal Growth from Melt–: Bridgman and Stockbargar, Czochralski and Vernuil methods. (ii) Crystal growth from liquid solution: Flux growth and temperature gradient methods (iii) Crystal growth from vapor phase: – Epitaxial growth methods.
		(c) Thin film preparation: Physical and Chemical methods.
		(d) Solid Solutions: Formation of Substitutional, Interstitial and Complex Solid Solutions; Mechanistic Approach; Study of Solid solutions by X-ray

		Powder Diffraction and Density Measurement.
	IV	1.4 Behaviour of Inorganic Solids (15 Lectures) (a) Diffusion in Solids: Fick's Laws of Diffusion; Kirkendal Effect; Wagner mechanism, Diffusion and Ionic Conductivity; Applications of Diffusion in Carburizing and non-Carburizing Processes in Steel Making.
		(b) Solid state reactions: General principles and factors influencing reactions of solids, Reactivity of solids.
		(c) Liquid Crystals: Introduction and classification of thermotropic liquid crystals, Polymorphism in liquid crystal, Properties and applications of liquid crystals.
		<u>REFERENCE BOOKS</u>
		<ol style="list-style-type: none"> 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 Ed., Cambridge University Press. 1997 4. L.V. Azaroff, Introduction to solids, Tata-McGraw Hill Book Co. New Delhi, 1977. 5. D.W. Bruce and Dermont O Hare, Inorganic Chemistry, 2nd Ed. Wiley and sons, New York, 1966. 6. J.M. Hollas, Symmetry in Molecules, Chapman and Hall Ltd., 1972. 7. Reboert L carter, Molecular Symmetry and Group Hohn Wiley and Sons, New York, 1988. 8. Ulrich Muller, Inorganic structural Chemistry, 2nd edition, John Wiley and Sons, Chichester, 1993. 9. R.N.Kutty and J.A.K.Tareen, Fundamentals of Crystal Chemistry, Universities Press (India) Ltd., 2001.. 10. 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. 11. D.K.Chakraborty, Solid State Chemistry, New Age International Publishers, 1996. 12. A. Earnshaw, Introduction to Magnetochemistry, Acad. Press, N.Y. (1966)
		2. Bioinorganic and Coordination Chemistry.
PSCHI 302	I	2.1 Bioinorganic Chemistry(15 Lectures) (i)Coordination geometry of the metal ion and functions. (ii)Zn in biological systems: Carbonic anhydrase, protolytic enzymes, e.g. carboxy peptidase, Zinc finger.

		(iii) Role of metal ions in biological electron transfer processes: iron sulphur proteins, (iv) Less common ions in biology e.g. Mn (arginase; structure and reactivity), Ni (urease ; structure and reactivity) (v) Biomineralization
	II	2.2 Reactivity of Chemical Species –I (15 Lectures) 2.2.1 Recapitulation of the definition of Lewis acids and bases, Classification of Lewis acids and bases based on frontier Molecular orbital topology, Reactivity matrix of Lewis acids and bases. 2.2.2 Group Characteristic of Lewis acids (Gp-1,13-17). 2.2.3 Pauling rules to determine the strength of oxoacids; classification and Structural anomalies.
	III	2.3 Reactivity of Chemical Species –II (15 Lectures) 2.3.1 Pourbaix Diagrams. 2.3.2 Amphoteric behavior, Periodic trends in amphoteric properties of p-block and d-block elements 2.3.3 Oxoanions and Oxocations. 2.3.4 Measures of hardness and Softness of Acids and Bases, Drago-wayland equations 2.3.5 Applications of acid-base Chemistry: Super acids and Super bases, heterogeneous acid-base reactions.
	IV	2.4 Structure, Bonding, and Stereochemistry of Coordination Compounds (15 Lectures) (a) Structure and Bonding. i) Molecular Orbital Theory for Complexes with Coordination Number 4 and 5 for the central ion (sigma as well as Pi bonding) (ii) Angular Overlap Model for octahedral and tetrahedral complexes for sigma and pi bond. (b) Stereochemistry of Coordination Compounds. (i) Chirality and Fluxionality of Coordination Compounds with Higher Coordination Numbers. (ii) Geometries of Coordination compounds from Coordination number 6 to 9.
		<u>REFERENCES:</u> 1. Gary Wulfsberg, Inorganic Chemistry ; Viva Books PA Ltd., New Delhi; 2002. 2. F.A. Cotton and Wilkinson, Advanced Inorganic Chemistry, 3 rd edition. 3. James E. Huheey, Inorganic Chemistry, 3 rd edition, Harper &

		<p>Row, Publishers, Asia, Pte Ltd., 1983.</p> <ol style="list-style-type: none"> 4. W.W.Porterfield, Inorganic Chemistry-An Unified Approach, Academic press(1993); 5. D.F.Shriver, P.W.Atkins and C.H. Langford, Inorganic Chemistry, 3rd edition Oxford University Press, 1999. 6. Asim K.Das, Fundamental Concepts of Inorganic Chemistry, (Volumes-I, II and III) CBS Pub.(2000) 7. N.N.Greenwood and A.Earnshaw, Chemistry of Elements, Pergamon, 1984. 8. J.M.Hollas, Symmetry in Chemistry, Chapmanad Hall Ltd., NY, 1972.\ 9. F.A.Cotton, Chemical Applications of Group Theory, 2nd edition, Wiley Eastern Ltd., New Delhi , 1976 10. C.J.Ballhausen and H.B.Gray, Molecular Orbital Theory, MCGraw-Hill, New York, 1965. 11. H. Sisler, Chemistry in Non-aqueous Solvents: New York Reinhold Publ. 1965. 12. . J.J. Lagowski, The Chemistry of Non-aqueous Solvents, Academic press, New york and London. 13. . C.M. Day and Joel Selbin, Theoretical Inorganic Chemistry, Affiliated East West Press Pvt.Ltd., 1985. 14. L.E.Orgel, An Introduction to Ligand Field Theory , Methuen & Co.Ltd., London, 1960. 15. F.Basolo and R.G.Pearson, Mechanisms of Inorganic Reactions, Wiley, New York, 1967. 16. . J.D.Lee, Concise Inorganic Chemistry, 5th ed., Blackwell ScienceLtd., 2005. 17. R.H. Crabtree, The Organometallic Chemistry of the Transition Metals, Wiley-Interscience, New york, 1988. 18. G.W.Parshall and S.D.Ittel, Homogeneous Catalysis, 2nd edition, John Wiley & sons, Inc., New York, 1992. 19. Gary O. Spessard and Gary L.Miessler, Organometallic Chemistry, Prentice-Hall, (1997). 20. . R.C.Mehrotra and A.Singh, Organometallic Chemistry-A Unified Approach, 2nd ed., New Age International Pvt.Ltd., 2000. 21. B.Douglas, D.H. McDaniel and J.J.Alexander, Concepts and Models of Inorganic Chmistry, 2nd edition, John Wiley & Sons, 1983. 22. James E.Huheey, Inorganic Chemistry-Principles of structure and reactivity, edn Harper & Row Publishers (1972). 23. . F. A. Cotton, G. Wilkinson, C. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th ed., John Wiley, New York, 1999. 24. F.A. Cotton and R.A.Walton, Multiple Bonds between Metal Atoms, 2nd edition, claranden Press, Oxford, 1993. 25. P.L. Soni, Vandana Soni , Ane Books Pvt., Ltd
		3. Spectral Methods in Inorganic Chemistry
I		3.1 Diffraction Methods –I (15 Lectures) X-Ray Diffraction: Bragg Condition; Miller

PSCHI 303		Indices; Laue Method; Bragg Method; Debye Scherrer Method of X-Ray Structural Analysis of Crystals.	
	II	3.2 Diffraction Methods –II (15 Lectures) (a) Electron Diffraction: Scattering of electrons, Scattering Intensity versus Scattering Angle, Weirl Measurement Technique, Elucidation of Structures of Simple gas Phase Molecules. (b) Neutron Diffraction: Scattering of Neutrons: Scattering of neutrons by Solids and Liquids, Magnetic Scattering, Measurement Technique.	
	III	3.3 Electron Spin Resonance Spectroscopy (15 Lectures) (a) Electron behaviour, interaction between electron spin and magnetic field. (b) Instrumentation : Source, Sample cavity. Magnet and Modulation coils, Microwave Bridge, Sensitivity. (c) Relaxation processes and Line width in ESR transitions: (i) ESR relaxation and chemical bonding. (ii) Interaction between nuclear spin and electron spin (hyperfine coupling) (iii) Spin polarization for atoms and transition metal ions, (iv) Spin-orbit coupling and significance of gtensors, (v) Application to transition metal complexes (having one unpaired electron)	
	3.4 Mossbauer Spectroscopy (15 Lectures)		
IV	Mössbauer Spectroscopy: 3.4.1 Basic principle, recoil energy and Doppler shift. 3.4.2 Instrumentation: sources and absorber; motion devices, detection, reference substances and calibration, 3.4.3 Isomer shift, quadrupole interaction, magnetic interaction, electronegativity and chemical shift. 3.4.4 Applications: <i>Iron compounds</i> - low spin and high spin Fe(II) and Fe(III) compounds and complexes, effect of pi-bonding, mono and poly nuclear Iron complexes, spinel oxides and iron-sulphur proteins; <i>Tin compounds</i> - tin halides and tin oxides, organotin compounds; <i>Iodine compounds</i> - I ₂ and alkali metal iodide compounds.		
		<u>REFERENCES:</u> 1. G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, Vogel's Textbook of Quantitative Chemical Analysis Fifth edition, (1996), ELBS Publication. Chapter 2, 3, 11. 2. W.H. Zachariasen. Theory of X-Ray Diffraction in Crystals. JohnWiley. New York. 1946.	

		<ol style="list-style-type: none"> 3. B.D. Cality,, Elements of X-Ray Diffraction Procedures. John Wiley and Sons. New York, 1954. 4. R. Reaching, Electron Diffraction, Methuen and Co. London. 1936 5. May and Leopold, An Introduction to Mossbauer Spectroscopy, Plenum, New York, 1971. 6. H.H. Willard, L.L. Merrit, J.A. Dean and F.A. Settle, Instrumental Methods of Analysis, C.B.S. Publishers and Distributors, New Delhi, 1986. 7. P.J. Horne, Nuclear Magnetic Resonance. Oxford University Press, Oxford, 1995. 8. Reverts John D., Nuclear Magnetic Resonance, McGraw Hill, New York, 1959. 9. . H. Kambe and P.D.Garn. Thermal Analysis, Kondansha Ltd. Toyo, 1974. 10. G.W. Ewing, Instrumental Methods, Of Analysis, 4th Ed. McFraw Hill Ltd., 1970. 11. N.H. Ring, Inorganic Polymers, Academic Press, New York, 1978 12. H.G. Heal, The Inorganic Heterocyclic Chemistry of Sulphur, Nitrogen and Phosphorous, Academic Press, New York, 1980. 13. G.T. Seaborg, Man-made Transuranic Elements Preitce- Hall, 1963. 14. M.T.R. Series, The Superheavy Elements. 15. Haissilsky, Nuclear Chemistry and its Application, 1962. 16. S. Glasstone, Sourcebook of Aomic Energy, East-West Publisher, 1969. 17. D.Harvey, Modern Analytical Chemistry, The McGraw-Hill Pub, 1st Edition(2000); 18. John H. Block, E.B. Roche, T.P. Soine and Charles O. Wilson, Inorganic Medicinal and Pharmaceutical Chemistry, Lea and Febiger, 1974. 19. R. S. Drago, Physical Methods in Inorganic Chemistry, John-Wiley Pub., 1975 20. . M. Drescher an G. Jeschke, (Eds), EPR Spetroscopy: Applications in Chemistry and Biology, Springer-Verlag Berlin, Heidelberg 2012 21. Graham Smith; David Keeble. Introduction to Modern EPR Spectroscopy CRC Press 2013. 22. C.N.R. Rao, Chemical Applications of Infrared Spectroscopy Academic Pess, N.Y. (1963) 23. K. Veera Reddy, Symmetry and Spectroscopy, 24. Paul Gabbott Principles and Applications of Thermal Analysis Wiley-Blackwell ; edition (2007) 25. . Richard Vernon Parish, NMR, NQR, EPR, and Mössbauer spectroscopy in inorganic chemistry, Publisher, E., Horwood, (1990)
		<p>4. Applied Chemistry (Elective)</p> <p>4.1 Safety in Chemistry Laboratories (15 Lectures)</p> <p>4.1.1 Handling of Hazardous Materials</p> <p>4.1.2 Toxic Materials (Various types of toxins and their effects on humans)</p>

PSCHI EC-I 304	I	4.1.3 Explosives and Inflammable Materials 4.1.4 Types of fire extinguishers(chemical reaction) 4.1.5 Bioactive materials. 4.1.6 Recycling& recovery of metals with reference to Silver, lead, cobalt, Nickel and chromium 4.1.7 Laboratory Wastes Disposal Management in Chemical Laboratories .
	II	4.2 Manufacture and Applications of Inorganic Compounds-I(15Lectures) 4.2.1 Lime, Chlorine and Caustic soda, 4.2.2 Ceramics and refractory materials 4.2.3 Cement 4.2.4 Inorganic explosives (mercury fulminate, Lead azide)
	III	4.3 Manufacture and Applications of Inorganic Compounds-II (15 Lectures) 4.3.1 Fertilizers and micronutrients 4.3.2 Glass 4.3.3 Paints and Pigments
	IV	4.4 Metallurgy (15 Lectures) 4.4.1 Occurrence, extraction and metallurgy of Zirconium, Hafnium, Niobium, Tantalum Platinum and Palladium metals. 4.4.2 Physical and chemical properties and applications of these metals, 4.4.3 Compounds of these metals, alloys and their uses.
		<u>REFERENCES:</u> <ol style="list-style-type: none"> 1. G.M.Masters, Introduction to Environmental Engineering and Science, Prentice-Hall of India Pvt. Ltd. New Delhi, 1995. 2. Sulabha K. Kulkarni, Nanotechnology-Principles and Practices, Capital Publishing Co., 2007. 3. K. R. Mahadik and B. S. Kuchekar, Concise Inorganic Pharmaceutical Chemistry, Nirali Prakashan, Pune, 19 . 4. D. A. Skoog, D. M. West, and F. J. Holler, Fundamentals of Analytical Chemistry, 7 th Edition, (printed in India in 2001), ISBN Publication. 5. B. Douglas, D.H. McDaniel and J. J. Alexander, Concepts and Models of Inorganic Chmistry, 2nd edition, John Wiley & Sons, 1983.
	I	4.1 Inorganic Materials (15 Lectures) Elective (a) Classification, manufacture and applications of (i) Inorganic fibers, and (ii) Inorganic fillers. Study of (i) Condensed phosphates, and (ii) Coordination polymers. (b) Preparation, properties and uses of industrially important chemicals – potassium permanganate, sodium thiosulphate, bleaching powder, hydrogen peroxide, potassium

PSCHI EC-II 304		dichromate
	II	<p>4.2 Nuclear Chemistry and Inorganic Pharmaceuticals (15 Lectures)</p> <p>(a) Nuclear Chemistry : Introduction to of nuclear fuels and separation of fission products from spent fuel rods by PUREX process. Super heavy element, discovery, preparation, position in the periodic table.</p> <p>(b) Inorganic Pharmaceuticals : Radiopharmaceuticals containing Tc and Bi, contrast agents for X-ray and NMR imaging. Gastrointestinal agents viz. (i) antacids(aluminium hydroxide, milk of magnesia, sodium bicarbonate and (ii) Cathartics(magnesium sulphate and sodium phosphate). Topical agents viz.(i) protectives and adsorbents(talc, calamine), (ii) antimicrobial agents(potassium permanganate, tincture iodine, boric acid) and astringents(potash alum) .</p>
	III	<p>4.3 Advances in Nanomaterials: (15 Lectures)</p> <p>(a) Types of nanomaterials, e.g. nanotubes, nanorods, solid spheres, core-shell Inanoparticles, mesoporous materials; isolation of nano materials</p> <p>(b) Some important properties of nanomaterials: optical properties of metal and semiconductor nanoparticles, magnetic properties.</p> <p>(c) Some special nanomaterials: Carbon nanotubes: Types, synthesis using various methods, growth mechanism, electronic structure; Porous silicon: Preparation and mechanism of porous silicon formation, Factors affecting porous structure, properties of porous silicon; Aerogels: Types of aerogels, Properties and applications of aerogels.</p> <p>(d) Applications of nanomaterials in electronics, energy, automobiles, sports and toys, textile, cosmetics, medicine, space and defense. Environmental effects of nanotechnology</p>
	IV	<p>4.4 Some Selected Topics (15 Lectures)</p> <p>i) Isopoly and Hetropoly acids, ii) Supramolecular chemistry iii) Inorganic pesticides, and iv) Intercalation compounds</p>
		<p style="text-align: center;"><u>REFERENCES:</u></p> <ol style="list-style-type: none"> 1. G.M.Masters, Introduction to Environmental Engineering and Science, Prentice-Hall of India Pvt. Ltd. New Delhi, 1995. 2. Sulabha K. Kulkarni, Nanotechnology-Principles and Practices, Capital Publishing Co., 2007. 3. K. R. Mahadik and B. S. Kuchekar, Concise Inorganic

- | | | |
|--|--|---|
| | | <p>Pharmaceutical Chemistry, Nirali Prakashan, Pune, 19 .</p> <p>4. D. A. Skoog, D. M. West, and F. J. Holler, Fundamentals of Analytical Chemistry, 7 th Edition, (printed in India in 2001), ISBN Publication.</p> <p>5. B.Douglas, D.H. McDaniel and J.J.Alexander, Concepts and Models of Inorganic Chmistry, 2nd edition, John Wiley & Sons, 1983.</p> |
|--|--|---|

**PRACTICALS
SEMESTER-III**

PSCHI3P1: Analysis of ores/alloys

1. Analysis of Brass alloy:
 - (i) Cu content by iodometric method,
 - (ii) Zn content by complexometric method.

2. Analysis of Mangelium alloy:
 - (i) Al content by gravimetric method as basic succinate,
 - (ii) Mg content by complexometric method.

3. Analysis of Bronze alloy:
 - (i) Cu content by complexometric method,
 - (ii) Sn content by gravimetric method.

4. Analysis of steel nickel alloy:
 - (i) Ni content by homogeneous precipitation method.

PSCHI3P2: Solvent Extraction

1. Separation of Mn and Fe using isoamyl alcohol and estimation of Mn
2. Separation of Co and Ni using n-butyl alcohol and estimation of Co
3. Separation of U and Fe using 8-hydroxyquinoline in chloroform and estimation of U
4. Separation of Fe and Mo using isoamyl alcohol and estimation of Mo
5. Separation of Cu and Fe using n-butyl acetate and estimation of Cu

PSCHI3P3: Inorganic Preparations

1. Preparation of V(oxinate)₃
2. Preparation of Sn(IV) Iodide
3. Preparation of Co(α -nitroso- β -naphthol)₃
4. Preparation of Ni(salicylaldoxime)₂
5. Hexamine cobalt (III) chloride
6. Preparation of Trans-bis (glycinato) Cu(II)

PSCHI3P4: Analysis of the following samples

1. Calcium tablet for its calcium content by complexometric titration.
2. Bleaching powder for its available chlorine content by iodometric method.
3. Iron tablet for its iron content colorimetry by 1,10-phenonthroline method.
4. Calcium tablet for its calcium content by complexometric titration.
5. Bleaching powder for its available chlorine content by iodometric method.
6. Iron tablet for its iron content colorimetry by 1,10-phenonthroline method.

7. Nycil powder for its Zn content complexometrically.

Reference books for practicals

1. A. I. Vogel, *Quantitative Inorganic Analysis*.
2. J. D. Woolins, *Inorganic Experiments*.
3. Palmer, *Inorganic Preparations*.
4. G. Raj, *Advanced Practical Inorganic Chemistry*.
5. J. E. House, *Inorganic chemistry*, Academic press, 2nd edition, (2013).

SEMESTER IV		
Course Code	Unit	Topics
		(Numericals and word problems wherever possible.)
PSCHI 401	I	<p>1 Properties of Inorganic Solids and Group Theory.</p> <p>1.1 Electrical Properties- (15 Lectures)</p> <p>(a) Electrical properties of solids: (i) Conductivity: Solid Electrolytes; Fast Ion Conductors; Mechanism of Conductivity; Hopping Conduction.</p> <p>(b) Other Electrical Properties: Thomson and Seebeck Effects; Thermocouples and their Applications; Hall Effect; Dielectric, Ferroelectric, Piezoelectric and Pyroelectric Materials and their Inter-relationships and Applications</p>
	II	<p>1.2 Magnetic Properties. (15 Lectures)</p> <p>(a) Behaviour of substances in magnetic field, mechanism of ferromagnetic and antiferromagnetic ordering , superexchange, 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.</p>
	III	<p>1.3 Thermal and Optical Properties (15 Lectures)</p> <p>a) Thermal Properties: Introduction, Heat Capacity and its Temperature Dependence; Thermal Expansion of Metals; Ceramics and Polymers and Thermal Stresses.</p> <p>(b) Optical properties: Color Centres and Birefringence; Luminescent and Phosphor Materials; Coordinate Model; Phosphor Model; Anti Stokes Phosphor; Ruby Laser; Neodymium Laser</p>
		1.4 Applications of group theory to –Electronic structures (15

	IV	<p>Lectures)</p> <p>(a) Recapitulation of Points groups and Character tables.</p> <p>(b) Transformation Properties of Atomic Orbitals;</p> <p>(c) Sigma and pi- molecular orbitals for AB₄ (tetrahedral) and AB₆ (octahedral) molecules;</p> <p>(d) Ligand Field Theory : Electronic structures of free atoms and ions; Splitting of levels and terms in a chemical environment; Construction of energy level diagrams; Direct product ; Correlation diagrams for d² ions in octahedral and tetrahedral ligand field; Methods of Ascending and Descending Symmetry; Hole formalism.</p>
		<p style="text-align: center;"><u>REFERENCE BOOKS</u></p> <ol style="list-style-type: none"> 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 Directons in Solid State Chemistry, 2nd Ed., Combridge University Press. 1997 4. L.V. Azaroff, Introductionn to solids, Tata-McGraw Hill Book Ce. New Dehli, 1977. 5. . D.W. Bruce and Dermont O Hare, Inorganic Chemistry, 2nd Ed. Wiely and sons, New York, 1966. 6. J.M. Hollas, Symmetry in Molecuies, Chapman adn Hall Ltd.,1972. 7. Reboert L carter, Molecular Symmeetry and Group Hohn Wiley and Sons, New York, 1988. 8. Ulrich Muller, Inorganic structural Chemistry, 2nd edition, John Wiley and Sons, Chichester, 1993. 9. . R.N.Kutty and J.A.K.Tareen, Fundamentals of Crystal Chemistry, Universities Press (India) Ltd., 2001.. 10. 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. 11. . D.K.Chakraborty, Solid State Chemistry, New Age International Publishers, 1996. 12. 12. A. Earnshaw, Introduction to Magnetochemistry, Acad. Press,N.Y. (1966)
	I	<p>2 Organometallics and main group Chemistry (15 Lectures)</p> <p>2.1 Organometallic Chemistry</p> <p>(a) Metal-Metal Bonding and Metal Clusters,</p> <p>(b) Electron Count and Structures of Clusters,,</p> <p>(c) Isolobal Analogy.</p> <p>(d)Organo Palladium and Organo Platinum Complexes (preparations, properties and applications.)</p> <hr/> <p>2.2 Applications of Organometallic Compounds (15 Lectures)</p>

PSCHI 402	II	(a) Catalysis-Homogenous and Heterogenous Catalysis: Comparison, Fundamental Reaction Steps. (b) Organometallics as Catalysts in Organic Reactions: (i)Hydrosilation, (ii)Hydroboratinn. (iii)_Water gas Shifts Reaction (iv) Wacker process(Oxidation of alkenes) (v)Alcohol corbonylation (c)Coupling reactions : (i) Heck's reaction (ii) Suzuki reaction
	III	2.3 Inorganic cluster and cage compounds (15 Lectures) (i) Introduction, (ii) Bonding in boranes, (iii) Heteroboranes, (iv) Carboranes, (v) cluster compounds, (vi) electron precise compounds and their relation to clusters.
	IV	2.4 Inorganic ring and chain compounds (15 Lectures) (a) Silicates, polysilicates and aluminosilicates, (b) Phosphazenes, phosphazene polymers (c) Polyanionic and polycationic compounds
		<u>REFERENCES:</u>
		<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. James E.Huheey, Inorganic Chemistry, 3rd edition, Harper & Row,Publishers, Asia, Pte Ltd., 1983. 4. W.W.Porterfield,Inorganic Chemistry-An Unified Approach,Academic press(1993); 5. D.F.Shriver, P.W.Atkins and C.H. Langford, Inorganic Chemistry,3rd edition Oxford University Press, 1999. 6. Asim K.Das, Fundamental Concepts of Inorganic Chemistry,(Volumes-I,II and III)CBS Pub.(2000) 7. N.N.Greenwood and A.Earnshaw, Chemistry of Elements, Pergamon, 1984. 8. J.M.Hollas, Symmetry in Chemistry, Chapmanad Hall Ltd., NY, 1972.\ 9. F.A.Cotton, Chemical Applications of Group Theory, 2nd edition, Wiley Eastern Ltd., New Delhi , 1976 10. C.J.Ballhausen and H.B.Gray, Molecular Orbital Theory, MCGraw-Hill, New York, 1965. 11. H. Sisler, Chemistry in Non-aqueous Solvents: New York Reinhold Publ. 1965. 12. . J.J. Lagowski, The Chemistry of Non-aqueous Solvents, Academic press, New york and London. 13. . C.M. Day and Joel Selbin, Theoretical Inorganic Chemistry,Affiliated East West Press Pvt.Ltd., 1985. 14. L.E.Orgel, An Introduction to Ligand Field Theory , Methuen &

		<p>Co.Ltd., London, 1960.</p> <p>15. F.Basolo and R.G.Pearson, Mechanisms of Inorganic Reactions, Wiley, New York, 1967.</p> <p>16. . J.D.Lee, Concise Inorganic Chemistry, 5th ed., Blackwell ScienceLtd., 2005.</p> <p>17. R.H. Crabtree, The Organometallic Chemistry of the Transition Metals, Wiley-Interscience, New york, 1988.</p> <p>18. G.W.Parshall and S.D.Ittel, Homogeneous Catalysis, 2nd edition, John Wiley & sons, Inc., New York, 1992.</p> <p>19. Gary O. Spessard and Gary L.Miessler, Organometallic Chemistry, Prentice-Hall, (1997).</p> <p>20. . R.C.Mehrotra and A.Singh, Organometallic Chemistry-A Unified Approach, 2nd ed., New Age International Pvt.Ltd., 2000.</p> <p>21. B.Douglas, D.H. McDaniel and J.J.Alexander, Concepts and Models of Inorganic Chmistry, 2nd edition, John Wiley & Sons, 1983.</p> <p>22. James E.Huheey, Inoganic Chemistry-Principles of structure and reactivity, edn Harper & Row Publishers (1972).</p> <p>23. . F. A. Cotton, G. Wilkinson, C. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th ed., John Wiley, New York, 1999.</p> <p>24. F.A. Cotton and R.A.Walton, Multiple Bonds between Metal Atoms, 2nd edition, claranden Press, Oxford, 1993.</p> <p>25. P.L. Soni, Vandana Soni ,Ane Books Pvt.,Ltd</p>
PSCHI 403	I	<p>3 Instrumental methods in Inorganic Chemistry .</p> <p>3.1 Spectroscopy (15 Lectures)</p> <p>(a) Infrared spectroscopy: Fundamental modes of vibrations, selection rules, IR absorption bands of metal - donor atom, effect of complexation on the IR spectrum of ligands formations on the IR of ligands like NH₃, CN⁻, CO, olefins (C=C) and C₂O₄²⁻ .</p> <p>(b) Raman spectroscopy: Raman spectroscopy for diatomic molecules. Determination of molecular structures like diatomic and triatomic molecules.</p>
		<p>(c) Applications of Group theory in Infrared and Raman spectroscopy.</p> <p>(c) Molecular Vibrations: Introduction; The Symmetry of Normal Vibrations; Determining the Symmetry Types of the Normal Modes; symmetry based Selection Rules of IR and Raman; Interpretation of IR and Raman Spectra for molecules such as H₂O, BF₃, N₂F₂, NH₃ and CH₄.</p>
		<p>(d) Nuclear Magnetic Resonance Spectroscopy :</p> <p>Introduction to basic principles and instrumentation. Use of ¹H, ¹⁹F, ³¹P, ¹¹B NMR spectra in structural elucidation of inorganic compounds; Spectra of paramagnetic materials: Contact shift, application of contact shift, lanthanide shift reagent.</p>
	II	<p>3.2 Microscopy of Surface Chemistry-I (15 Lectures)</p> <p>Introduction to surface spectroscopy, Microscopy, problems of surface analysis, distinction of surface species, sputter etching and depth profile and chemical imaging, instrumentations, Ion Scattering Spectra (ISS), Secondary Ion Mass Spectroscopy (SIMS), Auger Emission Spectroscopy</p>

		(AES),
	III	3.3 Microscopy of Surface Chemistry-II (15 Lectures) ESCA, Scanning Electron Microscopy (SEM), Atomic force microscopy (AFM) and transmission electron microscopy (TEM): Instrumentation and applications.
	IV	3.4 Thermal Methods (15 Lectures) 3.4.1 Application of TGA in Thermal characterization of polymers, quantitative analysis of mixture of oxalates, moisture content in coal, study of oxidation state of alloys etc. 3.4.2 Application of DSC and DTA in determination of thermodynamic parameters such as heat capacity and standard enthalpy of formation of the compounds, investigation of phase transitions, thermal stability of polymeric materials, purity of pharmaceuticals samples, M.P. and B.P. of organic compounds etc. 3.4.3 Basic principle, instrumentation and applications to other thermal methods like Thermomechanical analysis (TMA) and evolved gas analysis (EGA).
		<u>REFERENCES:</u>
		<ol style="list-style-type: none"> 1. G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, Vogel's Textbook of Quantitative Chemical Analysis Fifth edition, (1996), ELBS Publication. Chapter 2, 3, 11. 2. W.H. Zachariasen. Theory of X-Ray Diffraction in Crystals. John Wiley. New York. 1946. 3. B.D. Cality,, Elements of X-Ray Diffraction Procedures. John Wiley and Sons. New York, 1954. 4. R. Reaching, Electron Diffraction, Methuen and Co. London. 1936 5. May and Leopold, An Introduction to Mossbauer Spectroscopy, Plenum, New York, 1971. 6. H.H. Willard, L.L. Merrit, J.A. Dean and F.A. Settle, Instrumental Methods of Analysis, C.B.S. Publishers and Distributors, New Delhi, 1986. 7. P.J. Horne, Nuclear Magnetic Resonance. Oxford University Press, Oxford, 1995. 8. Reverts John D., Nuclear Magnetic Resonance, McGraw Hill, New York, 1959. 9. . H. Kambe and P.D.Garn. Thermal Analysis, Kondansha Ltd. Toyo, 1974. 10. G.W. Ewing, Instrumental Methods, Of Analysis, 4th Ed. McFraw Hill Ltd., 1970. 11. N.H. Ring, Inorganic Polymers, Academic Press, New York, 1978 12. H.G. Heal, The Inorganic Heterocyclic Chemistry of Sulphur, Nitrogen and Phosphorous, Academic Press, New York, 1980. 13. G.T. Seaborg, Man-made Transuranic Elements Preitce- Hall, 1963. 14. M.T.R. Series, The Superheavy Elements.

		<p>15. Haissilsky, Nuclear Chemistry and its Application, 1962.</p> <p>16. S. Glasstone, Sourcebook of Atomic Energy, East-West Publisher, 1969.</p> <p>17. D. Harvey, Modern Analytical Chemistry, The McGraw-Hill Pub, 1st Edition (2000);</p> <p>18. John H. Block, E.B. Roche, T.P. Soine and Charles O. Wilson, Inorganic Medicinal and Pharmaceutical Chemistry, Lea and Febiger, 1974.</p> <p>19. R. S. Drago, Physical Methods in Inorganic Chemistry, John-Wiley Pub., 1975</p> <p>20. . M. Drescher and G. Jeschke, (Eds), EPR Spectroscopy: Applications in Chemistry and Biology, Springer-Verlag Berlin, Heidelberg 2012</p> <p>21. Graham Smith; David Keeble. Introduction to Modern EPR Spectroscopy CRC Press 2013.</p> <p>22. C.N.R. Rao, Chemical Applications of Infrared Spectroscopy Academic Press, N.Y. (1963)</p> <p>23. K. Veera Reddy, Symmetry and Spectroscopy,</p> <p>24. Paul Gabbott Principles and Applications of Thermal Analysis Wiley-Blackwell ; edition (2007)</p> <p>25. . Richard Vernon Parish, NMR, NQR, EPR, and Mössbauer spectroscopy in inorganic chemistry, Publisher, E., Horwood, (1990)</p>
--	--	---

Course Code: PSCHIOC-I 404
Paper – IV (INTELLECTUAL PROPERTY RIGHTS & CHEMINFORMATICS)

Unit 1:	[15L]
Introduction to Intellectual Property:	[2L]
[2L]	
Historical Perspective, Different types of IP, Importance of protecting IP.	
Patents:	[5L]
[5L]	
Historical Perspective, Basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Health care-balancing promoting innovation with public health, Software patents and their importance for India.	
Industrial Designs:	[2L]
[2L]	
Definition, How to obtain, features, International design registration.	
Copyrights:	[2L]

[2L]

Introduction, How to obtain, Differences from Patents.

Trade Marks:

[2L]

[2L]

Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc.

Geographical Indications:

[2L]

[2L]

Definition, rules for registration, prevention of illegal exploitation, importance to India.

Unit 2:

[15L]

[15L]

Trade Secrets:

[2L]

[2L]

Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.

IP Infringement issue and enforcement:

[2L]

[2L]

Role of Judiciary, Role of law enforcement agencies – Police, Customs etc.

Economic Value of Intellectual Property:

[2L]

[5L]

Intangible assets and their valuation, Intellectual Property in the Indian context – Various Laws in India Licensing and Technology transfer.

Different International agreements:

[6L]

(a) World Trade Organization (WTO):

[5L]

- (i) General Agreement on Tariffs and Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement

(ii) General Agreement on Trade Related Services (GATS) Madrid Protocol.

(iii) Berne Convention

(iv) Budapest Treaty

(b) Paris Convention

[6L]

WIPO and TRIPS, IPR and Plant Breeders Rights, IPR and Biodiversity.

Unit III:

[15L]

[15L]

Introduction to Cheminformatics:

[5L]

[5L]

History and evolution of cheminformatics, Use of Cheminformatics, Prospects of cheminformatics, Molecular modeling and structure elucidation.

Representation of molecules and chemical reactions:

[5L]

[5L]

Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.

Searching Chemical Structures:

[5L]

[5L]

Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization.

Unit IV:

[15L]

[15L]

Applications:

Prediction of Properties of Compound, Linear Free Energy Relations, Quantitative Structure – Property Relations, Descriptor Analysis, Model Building, Modeling Toxicity, Structure – Spectra correlations, Prediction NMR, IR and Mass spectra, Computer Assisted Structure elucidations, Computer assisted Synthesis Design, Introduction to drug design, Target Identification and Validation, Lead Finding and Optimization, analysis of HTS data, Virtual Screening, Design of Combinatorial

Libraries, Ligand-based and Structure based Drug design, Application of Cheminformatics in Drug Design.

REFERENCES:

1. Andrew R. Leach & Valerie J. Gillet (2007) *An Introduction to Cheminformatics*. Springer: The Netherlands.
2. Gasteiger, J. & Engel, T. (2003) *Cheminformatics: A textbook*. Wiley-VCH
3. Gupta, S. P. *QSAR and Molecular Modeling*. Springer-Anamaya Pub.: New Delhi.

Course Code: PSCHIOC-II 404

PAPER – IV: RESEARCH METHODOLOGY

Unit 1:

[15L]

Print:

[5L]

Primary, Secondary and Tertiary sources.

Journals:

Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, textbooks, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.

Digital:

[5L]

Web sources, E-journals, Journal access, TOC alerts, Hot articles, Citation Index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups and communities, Blogs, preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki-databases, ChemSpider, Science Direct, SciFinder, Scopus.

Information Technology and Library Resources:

[5L]

The Internet and World wide web, Internet resources for Chemistry, finding and citing

published information.

Unit II: DATA ANALYSIS

[15L]

The Investigative Approach:

Making and recording Measurements, SI units and their use, Scientific methods and design of experiments.

Analysis and Presentation of Data:

Descriptive statistics, choosing and using statistical tests, Chemometrics, Analysis of Variance (ANOVA), Correlation and regression, curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, general polynomial fitting, linearizing transformations, exponential function fit, r and its abuse, basic aspects of multiple linear regression analysis.

Unit III: METHODS OF SCIENTIFIC RESEARCH AND WRITING SCIENTIFIC PAPERS

[15L]

Reporting practical and project work, Writing literature surveys and reviews, organizing a poster display, giving an oral presentation.

Writing Scientific Papers:

Justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work, writing ethics, avoiding plagiarism.

Unit IV: CHEMICAL SAFETY & ETHICAL HANDLING OF CHEMICALS

[15L]

Safe working procedure and protective environment, protective apparel, emergency procedure, first aid, laboratory ventilation, safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric pressure, safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals

in the sanitary sewer system, incineration and transportation of hazardous chemicals.

REFERENCES:

1. Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J., & Jones, A., (2011), *Practical skills in Chemistry*, 2nd Ed., Prentice Hall, Harlow.
2. Hibbert, D. B. & Gooding, J. J. (2006) *Data Analysis for Chemistry* Oxford University Press.
3. Topping, J., (1984) *Errors of Observation and their Treatment* 4th Ed., Chapman Hill, London.
4. Harris, D. C. (2007) *Quantative Chemical Analysis* 6th Ed., Freeman Chapters 3-5
5. Levie, R. De. (2001) *How to use Excel in Analytical Chemistry and in general scientific data analysis* Cambridge Universty Press.
6. Chemical Safety matters – IUPAC-IPCS, (1992) Cambridge University Press.
7. OSU Safety manual 1.01

PRACTICALS SEMESTER-IV

PSCHI4P1: Analysis of Ores

1. Analysis of galena ore:
 - (i) Pb content as PbCrO₄ by gravimetric method using 5% potassium chromate,
 - (ii) Fe content by colorimetrically using 1, 10- phenonthroline.
2. Analysis of Zinc blend ore:
 - (i) Zn content by complexometric method,
 - (ii) Fe content by colorimetric method (Azide method).
3. Analysis of Pyrolusite ore:
 - (i) Mn content by complexometric method,
 - (ii) Acid insoluble residue by gravimetric method.

PSCHI4P2: Coordination Chemistry

1. Determiation of Stability constant of $[\text{Zn}(\text{NH}_3)_4]^{2+}$ by potentiometry
2. Determiation of Stability constant of $[\text{Ag}(\text{en})]^+$ by potentiometry
3. Determiation of Stability constant of $[\text{Fe}(\text{SCN})]^{2+}$ by slope ratio method
4. Determiation of CFSE values of hexa-aqua complexes of Ti^{3+} and Cr^{3+} .
5. Determiation of Racah parameters for complex $[\text{Ni}(\text{H}_2\text{O})_6]^{2+}$ and $[\text{Ni}(\text{en})_3]^{2+}$

PSCHI4P3: Analysis of the following samples

1. Electral powder for Na/K content flame photometrically.
2. Fasting salt for chloride content conductometrically.
3. Sea water for percentage salinity by Volhard's method.
4. Soil for mixed oxide content by gravimetric method.
5. Fertilizer for potassium content by flame photometry.

PSCHI4P4: Project Evaluation & Spectral interpretation

Reference books for practicals	
1.	A. I. Vogel, <i>Quantitative Inorganic Analysis</i> .
2.	J. D. Woolins, <i>Inorganic Experiments</i> .
3.	Palmer, <i>Inorganic Preparations</i> .
4.	G. Raj, <i>Advanced Practical Inorganic Chemistry</i> .
5.	J. E. House, <i>Inorganic chemistry</i> , Academic press, 2 nd edition, (2013).