

**CY- 581**

**Frontiers in Physical Chemistry**

- 1. Statistical Thermodynamics:** Boltzmann distribution; kinetic theory of gases; partition functions and their relation to thermodynamic quantities – calculations for model systems.
- 2. Electrochemistry :** Nernst equation, redox systems, electrochemical cells; Debye Huckel theory; electrolytic conductance – Kohlrausch's law and its applications; ionic equilibria; conductometric and potentiometric titrations.
- 3. Solid State:** Crystal structures; Bragg's law and applications; band structure of solids.
- 4. Nuclear Chemistry:** Nuclear reactions, Fission and fusion, radio-analytical techniques and activation analysis.
- 5. Polymer Chemistry:** Molar masses, Kinetics of polymerization.

**REFERENCES:**

1. Concepts and Model of Inorganic Chemistry, B. Douglas, John Wiley & Sons, 3<sup>rd</sup> Ed. 2001.
2. Inorganic Chemistry, D. F. Shriver and P. W. Atkins, Oxford University, 4<sup>th</sup> Ed. 2006.
3. Inorganic Chemistry, J. E. Huheey, Pearson, 4<sup>th</sup> Ed. 2005.
4. Organic Synthesis - The Disconnection Approach, S.Warren, Willey Interscience, Ed. 1982.
5. Physical Chemistry, P. Atkins and J. D. Paula, Oxford, Ed. 2007.
6. Thermodynamics, Statistical Thermodynamics, and Kinetics, T. Engel and P. Reid, Prentice Hall, Ed. 2006.

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## CY-664 Interdisciplinary Topics in Chemistry

- 1. Nanoscience & Nanotechnology:-** Introduction of nanoscience and nanotechnology, Methods of generation of Nanomaterials, Methods of characterization of nanomaterials, Electron Microscope, XRD, Spectroscopic techniques, Properties and applications of Nanomaterials.
- 2. Green Chemistry:-** Introduction, the need of green chemistry, principles of green chemistry, sustainability, atom economy, E-factor, Role of catalyst, solvent, planning of green synthesis, tools of green chemistry, Green reactions, Aldol condensation, Cannizaro reaction and Grignard reaction- comparison of the above with classical reactions- Green preparations, enzymes and other alternate methods of synthesis in green chemistry.
- 3. Environmental Science:-** Composition of atmosphere, Chemical and photochemical reactions in the atmosphere, Ozone chemistry, Greenhouse effect, Global Warming, Types of pollution their monitoring and control.
- 4. Catalysis:-** Types of catalyst, Reactions, Catalyst synthesis, Catalyst deactivation & regeneration. Various Characterization techniques, industrial catalytic processes, Organometallics in homogenous catalysis.
- 5. Supra Molecular Chemistry:** Introduction to supra molecular chemistry, molecular forces, common supra molecules, experimental techniques in supra molecular chemistry, host / guest chemistry, molecular recognition- molecular receptors for different types of molecules including arisonic substrates, supra molecular design strategy & nanotechnology. Supramolecular devices. Supramolecular photochemistry.

### REFERENCES:

1. Principles of Nanoscience and Nanotechnology, M. A. Shah and Tokker Ahmed, Narosa Publication, Ed. 2011.
2. Nanotechnology Principles and Practices, Sulabha K. Kulkarni, Capital Publication, Ed. 2011.
3. Introduction to Nanotechnology, Charles P. Poole and Frank J. Owens, John Wiley & Sons, Ed. 2003.
4. Green Chemistry: Environment Friendly Alternatives, R Sanghi and M. M. Srivastava, Narosa Publication, Ed. 2009.
5. Green Chemistry: Greener Alternatives to Synthetic Organic Transformations, V. K. Ahluwalia, Narosa Publication, Ed. 2011.
6. Catalysis: Principles and Applications, B. Viswannathan, S. Sivasanker and A. V. Ramaswamy, Narosa Publication, Ed. 2007.

7. Catalysts and Surfaces: Characterisation Techniques, B. Viswannathan S. Kannan and R. C. Dekha, Narosa Publication, Ed. 2010.
8. Environmental Chemistry, B. K. Sharma and H. Kaur, Goel Publishing House, Ed. 1994.
9. Environmental Pollution Analysis, S. M. Khopkar, Wiley Eastern Ltd., Ed. 1995.
10. Supramolecular Chemistry – Fundamentals and Application, Katsuhiko Ariga and Toyoki Kunitake, Springer, 1<sup>st</sup> Ed. 2006.
11. Green Chemistry, P. T. Anastas and J. C. Warner, Oxford University Press, Ed. 1988.

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**CY- 653**

**Statistical Thermodynamics**

- 1. Generalized Coordinates of Phase Space:** Phase Space, density distribution in phase space, Liouville's Theorem, Microcanonical ensemble, Postulates of equal probabilities
- 2. The Classical Distribution Law:** Maxwell's Boltzmann Distribution Law, Maxwell's law of distribution of velocities, Principle of Equipartition of Energy
- 3. Introduction to Quantum Statistics:** Bose Einstein Statistics, Fermi Dirac Statistics, Maxwell Boltzmann Statistics, comparison of Bose Einstein, Fermi Dirac and Maxwell Boltzmann Statistics
- 4. Thermodynamics and Statistics:** Entropy and Probability, Entropy and number of eigen states, Thermodynamics of a Monoatomic Gas
- 5. Partition Function:** Partition function and Thermodynamic Properties, Translational Partition Function, Sackur-Tatode Equation, Separation of Internal Partition Function, rotational and Vibrational Partition Function
- 6. Applications of Partition Function:** Determination of thermodynamic properties, Ortho and Para hydrogen, free energy functions, Equilibrium Constant, effect of nuclear spin, Isomolecular reactions
- 7. Non-equilibrium Thermodynamics:** General Theory of non-equilibrium thermodynamics, entropy production in heat flow, matter flow and electric current, Onsager's reciprocal relations

**REFERENCES:**

- Physical Chemistry*, P. Atkins, J. D. Paula, Indian Edition, Oxford, **2007**.
- Thermodynamics, Statistical Thermodynamics, and Kinetics*, T. Engel and P. Reid, Prentice Hall, **2006**.
- Thermodynamics, A Core Course 3<sup>rd</sup> Edition* R. C. Srivastava, S. K. Saha, A. K. Jain, Prentice Hall of India, **2007**.
- Physical Chemistry*, T. Engel and P. Reid, Prentice Hall, **2006**.
- Theoretical Chemistry*, Samuel Glasstone, Wiley
- Non-equilibrium Thermodynamics, Principles and Applications* C. Kalidas, M. V. Sangaranarayanan Macmillan India Ltd., **2002**.

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CY-681

### Mechanistic Inorganic Chemistry

1. **Ligand Substitution** : Thermodynamic & Kinetic Aspects, Classification of Mechanisms.
2. **Ligand substitution in Square Planar Environment** : Nucleophilicity shape of transition state, examples.
3. **Ligand Substitution in Octahedral Environment** : Rate Laws, Activation, Stereochemistry and Isomerisation.
4. **Redox Reactions** : Classification, Inner sphere & Outer sphere mechanisms.
5. **Photochemical Reactions** : Prompt & delayed reactions metal-metal bond systems, d-d & charge transfer reactions.
6. **Catalysis** : Heterogeneous, Homogeneous catalysis and their important consequences.

#### REFERENCES :

1. *Inorganic Reaction Mechanism*, M. L. Tobe & J. Burgess, Longman, **1999**.
2. *Kinetics & Mechanism of Reactions of Transition Metals Complexes*, VCH, **1991**.
3. *Redox Mechanism in Inorganic Chemistry*, A. G. Lappin, E. Horwood, **1994**.
4. *Coordination Chemistry Reviews*, 249, **2005**.
5. *Mechanisms of Inorganic Chemistry*, F. Basolo and R. G. Pearson Wiley, **1967**.

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Prepared By: Dr. Sangeeta Obrai  
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- 1. Metal and Non-metal mediated oxidation and reductions:** Mechanism, selectivity, stereochemistry and applications of Chromium, Manganese, Silver, Ruthenium, DMSO, TEMPO, and iodine based reagents (IBX, Dess-Martion Periodinate); DDQ, Swern oxidation, Pd, S and Se catalysed dehydrogenation. Mechanism, selectivity, stereochemistry and applications of catalytic hydrogenations using Pd, Pt and Ni catalysts, Clemmensen reduction, Wolff-Kishner reduction, Dissolving metal reductions, metal hydride reductions using DIBAL. Boron in reduction.  
(10 Lectures)
- 2. Rearrangements:** A detailed study of the following rearrangements: Benzil-Benzilic acid, Arndt-Eister syntheses, Neber rearrangement, Shapiro reaction, Carroll, Gabriel–Colman, Smiles rearrangement, Stevens and Sommelet–Hauser rearrangements.  
(10 Lectures)
- 3. Reagents in organic synthesis:** Gilman's reagent, Lithium diisopropylamide (LDA), Dicyclohexyl Carbodiimide (DDC), 1,3-Dithiane (Umpolung reagent), Trimethylsilyliodide, Bakers yeast, Prevost Hydroxylation, Merifield resin, Ziegler-Natta catalyst, Lawson reagents, K-selecteride and L-selecteride, Sodium cyanoborohydride, 9-BBN, Manganese dioxide, Dioxiranes, Ceric ammonium nitrate, Tebbe reagent, Corey-Nicolaou reagent, Mosher's reagent. Use of Cu, B, Mg, Li, Zn, Si, Os, Ru, and Ti reagents inorganic synthesis.  
(10 Lectures)
- 4. New Synthetic Reactions:** Baylis-Hillman reaction, Biginelli reaction, Mukaiyama aldol reaction, Mitsunobu reaction, McMurrey reaction, Julia-Lythgoe olefination, and Peterson's olefination, Buchwald-Hartwig coupling, Shapiro reaction, Stork-enamine reaction Aza-Cope, Aza-Wittig reaction, BINAL and BINAP assisted reactions. Ugi reaction, Robinson–Gabriel synthesis, Strecker amino acid synthesis, Vilsmeier–Haack reaction, Wohl–Ziegler reaction.  
(10 lectures)

**References:**

- 1.Organic chemistry, Claydon, J., Gleaves, N., Warren, S., Wother, P.; (2001), Oxford University Press, UK.
- 2.Name Reactions: A Collection of Detailed Reaction Mechanism, Li, J.J., (2009). Springer, 4th edition.
- 3.Advanced organic chemistry: Reaction Mechanism, Bruckner, R., (2001). Elsevier, 1<sup>st</sup>edition.
- 4.Advanced Organic Chemistry Part A and Part B Carey, B. F. A., Sundberg R. J., (2007). Springer, 5th edition.
- 5.Some Modern Methods of Organic Synthesis, Carruthers, W., (2004). Cambridge Uni.Press, 4th edition.

6. Organic Synthesis: Special Techniques, Ahluwalia, V. K., Aggarwal R., (2001). Alpha Science, New Delhi.
7. Reagents for organic synthesis, Fieser and Fieser, (2011). Vol 1-26. Wiley Interscience, 3rd edition.
8. Organic Chemistry, Finar, I. L., (2012). Pearson Education, 6th edition, UK.
9. A text book of Organic Chemistry, Bansal, R.K., (2012). New Age International (P) Ltd., 4th edition New Delhi.
10. Advanced Organic Chemistry, Reactions Mechanisms and Structure, March, J., (2007) John Wiley, 6th edition.
11. Handbook of Reagents for Organic Synthesis Acidic and Basic Reagents Vol I. Reich, H. J., Rigby, M., (1999). IV Wiley-Interscience
12. Organic synthesis: The Synthon Approach. Warren, S., (2010). John Wiley & Sons, New York.
13. Designing organic synthesis: A Disconnection Approach Warren, S., (2010).. John Wiley and Sons, New York.

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