DISCIPLINE-SPECIFIC CORE COURSE - 20 (DSC-20)

Advanced Chemistry-II

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical		
Advanced Chemistry-II (DSC-20)	**04**	**03**	—	**01**	--	--

Learning Objective:

- This course delves into the fascinating intersection of bio-inorganic metals and their crucial roles in living systems. The detailed investigation of bio-inorganic chemistry of essential elements towards biomedical applications. To facilitate chemical transformations by providing the necessary conditions and catalysis.
- To provide a brief foundational understanding of the core principles of classical and quantum statistical mechanics.
- To explore the connection between macroscopic thermodynamics and microscopic quantum mechanics using various statistical ensembles.
- To introduce the Maxwell-Boltzmann, Bose-Einstein, and Fermi-Dirac statistics with a brief, qualitative understanding and focus on their applications.
- To enable students to apply statistical concepts in key areas such as the standard model for macromolecular systems, chemical kinetics, and chemical equilibrium.

Learning outcomes

By the end of the course, students will be able to:

- Understand the fundamental principles of statistical mechanics, including how they link microscopic behaviour to macroscopic properties of systems.
- Apply the Boltzmann distribution, Bose-Einstein statistics, and Fermi-Dirac statistics to various physical and chemical systems.
- Utilize partition functions to analyze and solve problems related to the thermodynamic properties of systems.
- Explore the application of statistical mechanics to key areas such as chemical kinetics, chemical equilibrium, and random walk models in macromolecular systems.
- Understand the advance application of bio-inorganic metals.

- Explore the structure and properties of inorganic materials used in biomedical applications.
- Investigate the biocompatibility and bioactivity of inorganic biomaterials.
- Discuss current research and future directions of bio-inorganic chemistry.
- Understand various reducing agents, oxidizing agents, and their applications in organic synthesis.
- Understand the conversion of specific functional groups without affecting others and maximize yields and selectivity for the desired products.

SYLLABUS OF DSC 20

Unit 1: Metals in Biological System **(Hours: 5)**

Biominerals and biomineralization, Detailed study of biocatalyst in the metabolism of Hydrogen, carbon, and sulfur, Biological actions of manganese, cobalt and nickel ions, Metal ions in brain and medicine, Homeostasis of Metals, Potassium-Dependent Molecules, Inorganic Nanoparticles in Wound Healing and Drug Delivery.

Unit 2: Inorganic Materials for Biomedical Applications **(Hours: 10)**

Natural Bone Structure and Composition, Calcium Phosphate Ceramics (e.g., hydroxyapatite, tricalcium phosphate), Metal Implants (e.g., titanium, stainless steel), Natural Tooth Structure and Composition (enamel, dentin), Dental Ceramics (e.g., zirconia, alumina), 3D Bioprinting.

Unit 3: *Reagents in Organic Synthesis* **(15 Hours)**

Triacetoxyborohydride, Lead Acetate, Phenyliodine (III) diacetate (PIDA), DCC, Tamao-Fleming Oxidation; Dimethyldioxirane (DMDO) Oxidation; DMSO (Barton modification &Swern Oxidation); Oxidation of organic compounds using thallium nitrate, selenium dioxide, phase transfer catalyst, crown ethers, $KMnO_4$, PCC, OsO_4, CrO_3, $K_2Cr_2O_7$.
Synthesis and applications of BuLi, Grignard, organoaluminium, and organozinc reagents. Applications of hydroboration (reductions, oxidations, and carbonylation): Diborane, 9-BBN.

Unit 4: Statistical Thermodynamics and its Applications **(15 Hours)**

Microstates, Configurations, coin tosses, rolling of dices, spin systems (in the absence of magnetic field),Thermodynamic probability, Stirling's approximation, Concepts of ensembles (Microcanonical and Canonical), Characteristic thermodynamic functions, Translational partition function (quantitative), Rotational and vibrational partition functions (qualitative), Maxwell-Boltzmann distribution, Bose-Einstein, and Fermi-Dirac Statistics (Qualitative).
Conventional transition state theory derived from partition functions, Equilibrium constants in terms of partition function: gas-phase reactions (K_p), isotope effects.
1-D random walk model, Number and weight average molecular weight, polydispersity index.

Practical Component

Identification of the product based on Melting point and spectroscopic techniques (IR, ^{1}HNMR, and ^{13}C NMR spectroscopy, data to be provided).

1. Synthesis and characterization of calcium phosphate ceramics spectrophotometrically /any other method.
2. Analyzing the composition of Bio materials(Stainless steel, hydroxyapatite)
3. Fabrication of a simple Bio-hydrogel (Polyvinyl alcoholhydrogel, polysaccharide hydrogel, cellulose,starch)
4. Preparation of Zirconia (ZrO_2).
5. Preparation and characterisation of transition metal complexes of riboflavin using commercially available Vitamin B2 supplements.
6. Synthesis of 1,2,3,4-tetrahydrocarbazole from cyclohexanone.
7. Reduction of *p*-nitrobenzaldehyde using suitable reagents. ($NaBH_4$/Sn-HCl)
8. Synthesis of 2,3-diphenylquinoxaline from benzil and *ortho*-phenylenediamine.
9. Oxidation of Aryl Aldehydes into Ester by I_2 and Alcohols.
10. Study the kinetics of the iodination of acetone in the presence of acid by the *Initial Rate Method*.
11. Titrate a tribasic acid (phosphoric acid) against NaOH and $Ba(OH)_2$ conductometrically.
12. Find the composition of the zinc ferrocyanide complex by potentiometric titration.
13. Statistical Treatment of Error Analysis (Null Hypothesis, T-test, F-test, Q-test (criteria for reject of hypothesis) Statistical analysis of laboratory data.
14. Determination of standard deviation, mean and maximum absolute errors, root-mean-square deviation (error) and Correlation coefficient of linear straight-line plot.

Recommended References and Textbooks (For Theory)

1. Bio-coordination Chemistry, D E Fenton, OUP, 2002
2. Principles of Bioinorganic Chemistry, S J Lippard and, J M Berg, USB, California, 1994
3. Biological Inorganic Chemistry, R.R Crichton, Elsevier, 2012
4. Y. Bar-Cohen, Biomimetics: Biologically Inspired Technologies, Taylor & Francis CRC Press, Boca Raton, FL, 2006.
5. R.L. Reis, S. Weiner, Learning from Nature How to Design New Implantable Biomaterials, Kluwer Academic Publishers, New York, 2005.
6. P. Behrens, E. Bäuerlein, Handbook of Biomineralization: Biomimetic and Bioinspired Chemistry, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2007.
7. H. Lowenstam, S. Weiner, On Biomineralization, Oxford University Press, New York, 1989.
8. S. Mann, Biomineralization: Principles and Concepts in Bioinorganic Materials Chemistry, Oxford University Press, Oxford, New York, 2001.
9. E. Bäuerlein, Biomineralization: Progress in Biology, Molecular Biology and Application, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2004.

10. E. Bäuerlein, Handbook of Biomineralization: Biological Aspects and Structure Formation, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2007.
11 F.E. Round, R.M. Crawford, D.G. Mann, The Diatoms: Biology and Morphology of the Genera, Cambridge University Press, Cambridge, 1990.
12 Carruthers, W. Modern Methods of Organic Synthesis. Cambridge University Press (**1996**).
13 Carey, F.A. & Sundberg, R. J. Advanced Organic Chemistry, Parts A & B, Plenum: U.S. (**2004**).
14 Jonathan Clayden, Nick Greeves, Stuart Warren. Organic Chemistry. Oxford. (**2000**).
15 McQuarrie, D. A. *Statistical Mechanics,* Viva Books Pvt. Ltd.: New Delhi (2003).
16 L. D. Landau and E. M. Lifshitz, Statistical Mechanics, Part I, Butterworth-Heinemann, 3rd ed. (2005).
17 Bagchi B. *Statistical Mechanics for Chemistry and Material Science,* CRC Press (2018).
18 Laidler, K. J. *Chemical Kinetics* 3rd Ed., Benjamin Cummings (1997).
19 Billmeyer, F. W. *Textbook of Polymer Science* 3rd Ed. Wiley-Interscience: New York (1984).
20 Pathria, R.K.; and Beale, P. D.;Statistical Mechanics, Fourth Edition, Elsevier, Academic press.
21 Huang, K., Statistical Mechanics, 2nd Ed., John Wley& Sons, New York (2000)

Recommended Reference and Textbooks (For Practical's)

1. Ahluwalia, V. K., Dhingra, S. (2004), Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press.
2. Ahluwalia, V. K., Aggarwal, R. (2004), Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press
3. Pasricha, S., Chaudhary, A. (2021), Practical Organic Chemistry: Volume–I, I K International Publishing house Pvt. Ltd, New Delhi
4. Pasricha, S., Chaudhary, A. (2021), Practical Organic Chemistry: Volume–II, I K International Publishing house Pvt. Ltd, New Delhi.
5. Khosla, B.D.; Garg, V.C.; Gulati, A. (2015), Senior Practical Physical Chemistry, R. Chand & Co, New Delhi.
6. McQuarrie, D. A. & Simon, J. D. *Physical Chemistry: A Molecular Approach* 3rd Ed., Univ. Science Books (2001).
7. Skoog, D. A.; Holler, F. J.; Crouch, S. R. Principles of Instrumental Analysis, Brooks/Cole Pub Co; 7th edition (1 January 2017).
8. Skoog, D. A.; West, D. M.; Holler, F. J.; Crouch, S. R. Fundamentals of Analytical Chemistry, Publisher: Holt, Rinehart & Winston of Canada Ltd; International 2 Revised ed edition (1 February 1988).