

**ACADEMIC AFFAIRS OFFICE
INDIAN INSTITUTE OF TECHNOLOGY ROORKEE**

No. Acd./²⁰³⁷~~2037~~/IAPC-78

Dated: January 21, 2020

Head, Department of Chemistry
(through e-mail)

The IAPC in its 78th meeting held on 31.12.2019 vide **Item No. 78.3.1** considered and approved the following courses:

1. PEC, CYN-308: Bioinorganic and Biomimetic Chemistry for Int. M.Sc. (Chemistry) III year. (**Appendix-A**)
2. OEC, ICY-305: Theoretical Aspects of Polymers (**Appendix-B**)


Assistant Registrar (Curriculum)

Encl: as above

Copy to (through e mail):-

1. All faculty
2. All Heads of Departments/ Centres
3. Dean, Academic Affairs
4. Associate Dean of Academic Affairs (Curriculum)
5. Channel I/ Academic webpage of iitr.ac.in

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: Department of Chemistry

1. Subject Code: CYN-308

Course Title: Bioinorganic and Biomimetic Chemistry

2. Contact Hours: L: 3

T: 0

P: 0

3. Examination Duration (Hrs.): Theory: 3

Practical: 0

4. Relative Weightage: CWS: 20-35

PRS: 0

MTE: 20-30

ETE: 40-50

PRE: 0

5. Credits: 3

6. Semester: Spring

7. Subject Area: PEC

8. Pre-requisite: Nil

9. Objective: To impart basic concepts of bioinorganic chemistry and its applications

10. Details of Course:

S. No.	Contents	Contact Hours
1.	Introduction: Origin of elements in biological systems. Essentials and trace metal ions. Biological ligands – Special ligands – porphyrins, chlorins, methnecorphan and corrin. Macromolecules – peptides and proteins, nucleic acids and nucleotides. Metal-DNA and RNA interactions – potential binding sites. Functions of metal ions in genetic regulations, replication, transcription and translation. Enzymes – Nomenclature and classification, kinetics of enzyme catalyzed reactions – Michaelis-Menten equation – effect of pH, temperature on enzyme reactions, factors contributing in the catalytic efficiency of enzymes and vitamin B₁₂ coenzyme– structure and reactions.	7
2.	Importance of alkali and alkaline earth metal-ions in biological systems: metal ion transport, membrane structure, ionophores, distribution of alkali metals and active transport of Na⁺ and K⁺ across biomembrane, calcium carriers – role of calcium in muscle contraction. Overview of heme proteins: Nomenclature of porphyrin system, substituent effects on porphyrin rings. Classification of heme proteins, natural oxygen carriers. Electron carriers: Cytochromes – introduction, classification. Iron-sulphur proteins – rubredoxin and ferridoxin, role of ferridoxins in mammalian respiratory system. Photosynthesis – chlorophylls, photosystem I and II. Model compounds for oxygen carriers – Vaska's complex, picket-fence porphyrins, cobalt Schiff-base complexes, complexes of copper with non-heme ligands.	10

3.	Non-redox reactions: Biological energy storage and transfer. Phosphate transfer and its activation by metal ions – phosphoryl transfer potential, phosphorylation – mechanism of phosphate transfer, hydrolysis. Beneficial and toxic effects of metal ion introduced externally: Medicinal – anti-cancer agents, inorganic radioisotopes in diagnosis and treatment. Bioorganometallic compounds as drugs and enzyme inhibitors. Metal ion poisoning: Toxicity of Hg, Cd, Pb and As; chelation therapy. Inorganic plant nutrition and indicator plants for mineral exploration.	9
4.	Biomimetics: Basics and importance of artificial photosynthesis; renewable energy through artificial photosynthesis - first, second and third generation solar cells; solar water splitting (photoelectrolysis) using various semiconductors; hydrogen fuel cells; industrial electrolyzers for water splitting; biomass to energy; solar CO₂ fixation; bioinspired catalysis, artificial enzymes and nanozymes; bioinspired and biomimetic materials; molecular recognition and sensing, transition metal complexes of dinitrogen and reduction of dinitrogen to ammonia.	16
Total		42

11. Suggested Books:

S. No.	Name of Books / Authors	Year of Publication
1.	Huheey, J.E., Keiter, E.; Keiter, R. and Medhi, O.K., "Inorganic Chemistry: Principles of Structure and Reactivity", 4 th Ed., Pearson Education Asia.	Reprint 2019
2.	Gibbs, W., "Concepts and Applied Principles of Bioinorganic Chemistry", Vol. I, II and III Callisto Reference, UK.	2015
3.	Lippard, S.J. and Berg, J., "Principles of Bioinorganic Chemistry", University Science Books, USA.	Reprint 2005
4.	Kaim, W., Schwederski, B. and Klein, A. "Bioinorganic Chemistry-Inorganic Elements in the Chemistry of Life: An Introduction and Guide", Wiley & Sons, Germany.	2013
5.	I. Bertini, H. B. Gray, E. I. Stiefel, and J. S. Valentine, "Biological Inorganic Chemistry: Structure and Reactivity" University Science Books, CA, USA.	2006
6.	Atkins, P., Overton, T., Rourke, J., Mark, W. and Armstrong, F., "Shriver and Atkins' Inorganic Chemistry", 5 th Ed, Oxford university press.	2011
7.	Kadish, K. M., Smith, K. M. and Guillard, R. "Handbook of Porphyrin Science", Vol. 12, World Scientific, Singapore.	2011

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT/CENTRE: Chemistry Department

1. **Subject code:** ICY-305 **Course Title:** Theoretical Aspects of Polymers
2. **Contact Hours:** **L:** 3 **T:** 0 **P:** 0
3. **Examination Duration (Hrs):** **Theory:** 3 **Practical:** 0
4. **Relative Weightage:** **CWS:** 20-35 **PRS:** 0 **MTE:** 20-30 **ETE:** 40-50 **PRE:** 0
5. **Credits:** 3 6. **Semester:** Spring /Autumn 7. **Subject Area:** OEC
8. **Pre-requisite:** NIL
9. **Objective:** To familiarize students with the basic theoretical concepts of polymers.

10. Details of the Course:

S. No.	Contents	Contact Hours
	Statistical Thermodynamics: Microstates, Ensembles-microcanonical, canonical, grand-canonical, Partition functions, distributions, Averages, thermodynamic connection, probability distribution of fluctuations	6
1.	Chain Statics: Characteristic dimensions of 'random coil' polymers, models for calculating the average end-to-end distance for an ensemble of statistical chains, distribution of end-to-end vectors, Worm-like chain, measurement of radius of gyration from scattering, free energy of ideal chain, scaling arguments for stretching and confinement, pair correlation for ideal chain, structure factor.	12
2.	Real chains: Excluded volume, self-avoiding walks, deforming real and ideal chains, scaling model for real chains, Flory theory, solvent quality, theta-temperature. Thermodynamics and statistical mechanics of polymer networks.	8
3.	Polymer solutions: Thermodynamics of mixing, Flory-Huggins theory, osmotic pressure, concentration regimes in polymer solutions, correlation length, correlation function, screening of excluded volume forces, size of a polymer in semi-dilute solutions, polymer-polymer blends and phase diagrams.	9
4.	Polymer melts: chains in melts, screening in dense polymer melts, correlation hole.	3
5.	Polymer dynamics: Rouse model, Zimm model, reptation	4
	Total	42

11. Suggested Books:

S. No.	Name of Authors/Book/ Publisher etc.	Year of Publication/ Reprint
1	Fredrickson G., "The Equilibrium Theory of Inhomogeneous Polymers", Oxford University Press.	2013
2	Kawakatsu T., "Statistical Physics of Polymers: An Introduction", Springer	2013
3	Doi M., Edwards S.F., "The Theory of Polymer Dynamics", The International Series of Monographs on Physics, vol. 73, Oxford: Clarendon Press.	2013
4	Gedde U., "Polymer Physics", ebook, Dordrecht: Springer Netherlands.	2013
5	Strobl G. R., "The Physics of Polymers: Concepts for Understanding Their Structures and Behavior", 3 rd Ed., Berlin; London : Springer.	2011
6	Flory P. J., "Principles of Polymer Chemistry", 1 st Ed. publ. 1953, 20 reprint, Ithaca: Cornell University Press.	2010
7	de Gennes P.G., "Scaling Concepts in Polymer Physics", 1 st Ed., Ithaca, NY: Cornell University Press.	2005
8	Rubinstein M., Colby R. C., "Polymer Physics", 1 st Ed., Oxford University Press.	2003