COURSE PLAN - CY1020

1. Course code and Title : CY1020; Thermodynamics, Kinetics and Organic Reactions

2. Course category : BST

3. Course credit : 2-1-0-3 (L-T-P-C)

4. Prerequisite course : Nil

5. Consent of Teacher : Not required

6. Learning Objectives :

This is a basic level course in chemistry that will promote the knowledge and application of Physical and Organic concepts in Chemistry amongst the engineering candidates and equip them with a utility tool before exploring their respective engineering streams. The main objective of this course is to expose the students to thermodynamics of microscopic and macroscopic systems, the rate (kinetics) of day to day processes and the structure, characteristics and reactions of organic systems.

7. Learning Outcomes : At the end of the course, the students should be able to

(i) Understand how thermodynamics and chemical kinetics are useful to chemists, for predicting the possibility of reactions, and understanding mechanism of reactions.
(ii) Describe the thermodynamic properties of pure substance and mixtures.
(iii) Use thermodynamic data to get information on equilibrium.
(iv) Explain the reactivity and stability of organic molecules.
(v) Understand and use HMO theory and 4n+2 rule.
(vi) Describe mechanisms for aromatic organic reactions, pericyclic reactions,
(vii) Design and synthesize aromatic compounds, and
(viii) Characterize organic systems using spectroscopic techniques.

8. Course content:

Chemical Thermodynamics: Laws of Thermodynamics, Entropy change accompanying various processes (isothermal expansion, phase transition, heating, entropy of mixing of perfect gases); Absolute entropy and the Third Law of thermodynamics; Statistical entropy; Spontaneity of a chemical reaction and Gibbs energy; Standard Gibbs energies of formation and reactions; Thermodynamic functions (A, G, U & H) and four fundamental equations, Maxwell relationships; variation of G with T and P, Gibbs-Helmholtz equation, Chemical potential; G versus extent of reaction, Equilibrium constant through chemical potential (gas equilibria), reaction between K_p & K_c.

Chemical Kinetics: Parallel, opposing and consecutive reactions; Mechanism of complex chemical reactions; Analysing mechanisms using the steady-state approximation, Chain reactions (hydrogen-bromine reaction); Unimolecular reactions (thermodynamic approach); Transition State Theory for bimolecular reactions (thermodynamic approach); Enzyme catalysis (Michaelis-Menten Mechanism).

Aromaticity: HMO Theory, aromatic, non-aromatic and anti-aromatic compounds. Basic concepts of NMR spectroscopy; ring current and diamagnetic anisotropy; applications.

Aromatic substitution reactions: Aromatic electrophilic substitution and Aromatic nucleophilic substitution reactions. Applications briefly: production of Ibuprofen and paracetamol. Application of Sangers reagent.

Pericyclic reactions: Definition, classifications, electrocyclic reaction of butadiene and hexatriene, photochemical [2+2] and thermal [4+2] cycloadditions, Sigmatropic rearrangements - limited to Cope and Claisen rearrangements, FMO approach - Woodward Hoffmann rules and basic stereochemistry aspects of

the above reactions.

9. Text books:

1. Organic Chemistry, Paula Y Bruice, 7th Edition, Springer, 2009, Pearson. ISBN-13: 978-0321819031
2. Organic Chemistry, Robert Thornton Morrison and Robert Neilson Boyd, 6th Edition, Pearson. ISBN 9788131704813
3. Introduction to spectroscopy, Pavia, 4th Edition, Science Publisher, 2015. ISBN: 9780495114789
4. Organic Chemistry by J Clayden, N Greeves and S Warren, 2nd Edition 2012, Oxford University Press. ISBN: 978-0199270293
5. Physical Chemistry, Peter Atkins and Julio de Paula, 10th Edition, Oxford University Press. ISBN: 9780199697403
6. Physical Chemistry – A Molecular Approach, Donald A McQuarie and John D Simon, Viva Books. ISBN10: 0935702997 ISBN13: 9780935702996
7. Fundamentals of Molecular Spectroscopy by C N Banwell and E M McCash, 4th Ed., Tata McGraw-Hill. ISBN:0077079760 9780077079765

10. Referance books:

1. Advanced Organic Chemistry, Part A by F. A. Cary and R. I. Sundberg, 5th Edition, Springer, 2009. ISBN 978-0-387-44899-2
2. Pericyclic Reactions, Ian Fleming, 2nd Edition 2015, Oxford Chemistry Primers. ISBN: 9780199680900
3. Physical Chemistry, R Stephen Berry, Stuart A Rice and John Ross, 2nd Edition 2007, Oxford University Press. ISBN: 9780195105896

Proposing Faculty :

Department / Centre : Chemistry

Proposal Type : Revised

Programme : B.Tech