MSc Chemistry

SEMESTER III

Core Papers	**SEC**	**Generic electives**
BCH-CC6 TH (4 C) BCH-CC6 PR (2 C)	SEC (2C) *Any two from SEC-1 to SEC-6*	GE3 (6 C) *option is available for 6 credit transfer from MOOCs/SWAYAM platform*
BCH-CC7 TH (4 C) BCH-CC7 PR (2 C)		

SEMESTER III
PHYSICAL CHEMISTRY II

PAPER CODE: BCH-CC06
PAPER TITLE: PHASE EQUILIBRIA AND CHEMICAL KINETICS

Total Credits: 06 - (BCH-CC06TH -04, BCH-CC06PR -02)
Total Lectures: BCH-CC06TH - 60, BCH-CC06PR -60

Objectives:

The core course Phase Equilibria and Chemical Kinetics is designed to strengthen the basic and fundamental concepts of physical Chemistry. The course is imbued with the applications of these concepts, the chemical equilibrium, phase equilibria, chemical kinetics and concepts of colligative properties are introduced.

Course Learning Objectives:

On completion of the course, the student will be able to:

CLO 1 Understand and explain the different nature and behavior of chemical and phase equilibria concepts learnt.(Cognitive level: Understand).

CLO 2 Learn and understand many concepts of degree of freedom, chemical kinetics and solution.(Cognitive level: learn and understand).

CLO 3 Solving many numerical problems related to prepare solution of different strength. (Cognitive level: Analyze and apply).

CLO 4 Derive fundamental and applied derivation of chemical equilibria, kinetics and phase equlibria.(Cognitive level: Apply).

CLO 5 Determination of molecular mass using colligative property.(Cognitive level: Determine).

Mapping of CLOs with PLOS

	CLO1	CLO 2	CLO 3	CLO 4	CLO 5
PLO1.	3	3	2	2	2
PLO2.	3	3	2	2	2
PLO3.	3	3	2	2	2
PLO4.	2	3	3	2	2
PLO5.	2	2	3	3	2
PLO6.	2	2	2	3	3
PLO7.	2	2	2	3	3
PSO1	3	3	2	2	2
PSO2	3	3	2	2	2
PSO3	3	3	3	2	2
PSO4	2	2	2	3	3
PSO5	2	2	3	3	2
PSO6	2	2	2	3	3
PSO7	2	2	2	3	3
PSO8	2	2	2	2	3
PSO9	2	2	2	2	3

3: High-level mapping, 2 - Medium-level mapping, 1 -Low-level mapping.

Core paper

PAPER CODE: BCH-CC6 TH
TITLE: PHASE EQUILIBRIA AND CHEMICAL KINETICS
PHYSICAL CHEMISTRY II
SEMESTER III

TOTAL HOURS: 60 **CREDITS: 04**

UNIT I: CHEMICAL EQUILIBRIUM [15 Hours]

Criteria of thermodynamic equilibrium, degree of advancement ofreaction, chemical equilibria in ideal gases. Thermodynamic derivation of relation between Gibbs free energy of reaction and reaction quotient. Equilibrium constants and their quantitative dependence on temperature, pressure and concentration (Le Chatelier Principle, Quantitatively)). Free energy of mixing and spontaneity. equilibrium between ideal gases and a pure condensed phase.

UNIT II: PHASE EQUILIBRIA [15 Hours]

Concept of phases, components and degrees of freedom, derivation of Gibbs Phase Rule fornon-reactive and reactive systems; Clausius-Clapeyron equation and its applications to solidliquid,liquid-vapour and solid-vapour equilibria, phase diagram for one component systems,with applications.Phase diagrams for systems of solid-liquid equilibria involving eutectic, congruent andincongruent melting points, solid solutions.

Three component systems, water-chloroform-acetic acid system, triangular plots.*Binary solutions:* Gibbs-Duhem-Margules equation, its derivation and applications tofractional distillation of binary miscible liquids (ideal and non-ideal), azeotropes, lever rule,partial miscibility of liquids, CST, miscible pairs, steam distillation.Nernst distribution law: its derivation and applications.

Unit III: CHEMICAL KINETICS [15 Hours]

Order and molecularity of a reaction, rate laws in terms of the advancement of a reaction,differential and integrated form of rate expressions up to second order reactions, experimentalmethods of the determination of rate laws, kinetics of complex reactions (integrated rateexpressions up to first order only): (i) Opposing reactions (ii) parallel reactions and (iii)consecutive reactions and their differential rate equations (steady-state approximation inreaction mechanisms) (iv) chain reactions.

Temperature dependence of reaction rates; Arrhenius equation; activation energy. Collisiontheory of reaction rates, Lindemann mechanism, qualitative treatment of the theory ofabsolute reaction rates.

UNIT IV: SOLUTIONS AND COLLIGATIVE PROPERTIES [15 Hours]

Dilute solutions; lowering of vapour pressure, Raoult's and Henry's Laws and their applications. Thermodynamic derivation using chemical potential to derive relations between the four colligative properties [(i) relative lowering of vapour pressure (ii) elevation of boiling point, (iii) Depression of freezing point, (iv) osmotic pressure] andamount of solute. Applications in calculating molar masses of normal, dissociated and associatedsolutes in solution.

Suggested Reading:

1. Peter Atkins & Julio De Paula, *Physical Chemistry* 10th Ed., Oxford University Press(2014).
2. Castellan, G. W. *Physical Chemistry*, 4th Ed., Narosa (2004).
3. McQuarrie, D. A. & Simon, J. D., *Molecular Thermodynamics*, Viva Books Pvt. Ltd.New Delhi (2004).
4. Engel, T. & Reid, P. *Physical Chemistry 3rd Ed.,* Prentice-Hall (2012).
5. Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S.*Commonly Asked Questions in Thermodynamics.* CRC Press: NY (2011).
6. Zundhal, S.S. *Chemistry concepts and applications* Cengage India (2011).
7. Ball, D. W. *Physical Chemistry* Cengage India (2012).
8. Mortimer, R. G. *Physical Chemistry 3rd Ed.,* Elsevier: NOIDA, UP (2009).
9. Levine, I. N. *Physical Chemistry 6th Ed.,* Tata McGraw-Hill (2011).
10. Metz, C. R. *Physical Chemistry 2nd Ed.*, Tata McGraw-Hill (2009).

Core paper

PAPER CODE: BCH-CC6 PR
TITLE: PHASE EQUILIBRIA AND CHEMICAL KINETICS
PHYSICAL CHEMISTRY- II
SEMESTER III

TOTAL HOURS: 60 **CREDITS: 02**

Phase Equibria:

I. Determination of critical solution temperature and composition at CST of the phenol water system and to study the effect of impurities of sodium chloride and succinic acid on it.
II. Phase equilibria: Construction of the phase diagram using cooling curves or ignition tubemethod: a. simple eutectic and b. congruently melting systems.
III. Distribution of acetic/ benzoic acid between water and chloroform or cyclohexane.
IV. Study the equilibrium of at least one of the following reactions by the distribution method:

a. $I_2(aq) + I^-(aq) \rightarrow I_3(aq)$
b. $Cu^{2+}(aq) + nNH_3 \rightarrow Cu(NH_3)_n^{2+}$

Potentiometry:

Perform the following potentiometric titrations: i. Strong acid vs. strong base ii. Weak acid vs. strong base iii. Dibasic acid vs. strong base iv. Potassium dichromate vs. Mohr's salt

Suggested Reading

- Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011). 25
- Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry 8th Ed.; McGraw-Hill: New York (2003).
- Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H.Freeman & Co.: New York (2003).

Teaching Learning Process:

- Lectures in classrooms
- Peer learning
- Hands-on learning using lab practicals, videos, presentations, seminars
- Technology-driven Learning

Assessment Methods:

- Continuous Evaluation: by monitoring the progress of student's learning
  - Class Tests, Worksheets and Quizzes
  - Presentations, assignments , Group discussions, projects, viva-voce to enhance critical thinking skills and personality
- Semester-end Examination: a critical indicator of student's learning and teaching methods adopted by teachers throughout the semester.

Keywords:

Phase Equilibria, Chemical Equilibrium, Chemical Kinetics, Solutions And Colligative Properties

SEMESTER III ORGANIC CHEMISTRY-II
PAPER CODE: BCH-CC07TH **PAPER TITLE: HALOGENS, OXYGEN AND NITROGEN CONTAINING FUNCTIONAL GROUPS**
Total Credits: 06 - (BCH-CC07TH -04, BCH-CC07PR -02) **Total Lectures: BCH-CC07TH - 60, BCH-CC07PR -60**

Objectives: The core course Organic chemistry-II is designed to strengthen the basic and fundamental concepts of functional groups and their characteristic physical and chemical properties. The course is permeated with the applications of these concepts of Halogens, Oxygen and Nitrogen containing functional groups, their identification, distinction, synthesis and reactivity concepts are introduced.

Course Learning Objectives:

On completion of the course, the student will be able to:

CLO 1. Understand and explain the different nature and behaviour of organic compounds based on fundamental concepts learnt. (Cognitive level: Understand).

CLO 2. Learn and understand many organic reaction mechanisms including Nucleophilic Substitution, Eliminations, Nucleophilic additions, Nucleophilic addition-Eliminations, Grignard reaction, applications of BuLi, Bouvaelt-Blanc Reduction, Pinacol-Pinacolone rearrangement, Oxidative cleavage of glycols by periodic acid and lead tetraacetate, Reimer–Tiemann and Kolbe's–Schmidt Reactions, Fries and Claisen rearrangement, Darzens epoxidation, Aldol & Benzoin condensation, Knoevenagel condensation, Claisen-Schmidt, Perkin, Cannizzaro reaction, Wittig reaction, haloform reaction, Beckmann rearrangement and Benzil-Benzilic acid rearrangement, Baeyer Villiger oxidation, Clemmensen reduction, Wolff-Kishner reduction, reductions using $LiAlH_4$, $NaBH_4$, MPV, PDC and PGC, Michael addition, Claisen condensation, Dieckmann and Reformatsky reactions, Hofmann Bromamide reaction,Curtius rearrangement, Gabriel phthalimide synthesis, Carbylamine reaction, Mannich reaction, Hoffmann's exhaustivemethylation, Hofmann-elimination reaction, Schotten Baumann reaction, Sandmeyer reaction, Balz-Schiemann reaction. (Cognitive level: Learn and Understand).

CLO 3. Formulate the mechanisms of organic reactions by recalling and correlating the fundamental properties of the reactants involved. (Cognitive level: Learn and Understand).

CLO 4. Use the fundamental reactivity concepts to identify and analyze reaction mechanisms including Nucleophilic addition, Substitution, Aromatic Nucleophilic substitution, functional group interconversions. (Cognitive level: Learn, Understand and analyze).

CLO 5. Practically apply the basic oxidation/reduction reactions for functional group transformations. (Cognitive level: Apply).

CLO 6. Apply the fundamental reactivity concepts to bring about chemical transformations in the laboratory and synthesize small molecules useful to society. (Cognitive level: Apply).

Mapping of CLOs with PLOS

	CLO1	CLO 2	CLO 3	CLO 4	CLO 5	CLO 6
PLO1.	**3**	**3**	**2**	**2**	**2**	**2**
PLO2.	**3**	**3**	**2**	**2**	**2**	**2**
PLO3.	**3**	**3**	**2**	**2**	**2**	**2**
PLO4.	**2**	**3**	**3**	**2**	**2**	**2**
PLO5.	**2**	**2**	**3**	**3**	**2**	**2**
PLO6.	**2**	**2**	**2**	**3**	**3**	**3**
PLO7.	**2**	**2**	**2**	**3**	**3**	**3**
PSO 1.	**3**	**3**	**2**	**2**	**2**	**2**
PSO 2.	**3**	**3**	**2**	**2**	**2**	**2**
PSO 3.	**3**	**3**	**3**	**2**	**2**	**2**
PSO 4.	**2**	**2**	**2**	**3**	**3**	**3**
PSO 5.	**2**	**2**	**3**	**3**	**2**	**2**
PSO 6.	**2**	**2**	**2**	**3**	**3**	**3**
PSO 7.	**2**	**2**	**2**	**3**	**3**	**3**
PSO 8.	**2**	**2**	**2**	**2**	**3**	**3**
PSO 9.	**2**	**2**	**2**	**2**	**3**	**3**

3: High-level mapping, 2 - Medium-level mapping, 1 -Low-level mapping.

Core Paper

SEMESTER III
PAPER CODE: BCH-CC7 TH
ORGANIC CHEMISTRY-II
TITLE: HALOGENS, OXYGEN AND NITROGEN CONTAINING FUNCTIONAL GROUPS

TOTAL HOURS: 60 **CREDITS: 04**

UNIT I: CHEMISTRY OF HALOGENATED HYDROCARBONS: [15 Hours]

Alkyl halides: Methods of preparation, nucleophilic substitution reactions – SN_1, SN_2 and SNi mechanisms with stereochemical aspects and effect of solvent etc.; nucleophilic substitution vs. elimination.
Aryl halides: Preparation, including preparation from diazonium salts. nucleophilic aromatic substitution; SNAr, Benzyne mechanism.
Relative reactivity of alkyl, allyl/benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.
Organometallic compounds of Mg and Li – Use in synthesis of organic compounds.

UNIT II: ALCOHOLS, PHENOLS, ETHERS AND EPOXIDES AND CARBONYL COMPUNDS [15 Hours]

Alcohols: preparation, properties and relative reactivity of 1°, 2°, 3° alcohols, Bouvaelt-Blanc Reduction; Preparation and properties of glycols: Oxidation by periodic acid and lead tetraacetate, Pinacol-Pinacolone rearrangement;
Phenols: Preparation and properties; Acidity and factors effecting it, Ring substitution reactions, Reimer–Tiemann and Kolbe's–Schmidt Reactions, Fries and Claisen rearrangements with mechanism;
Ethers and Epoxides: Preparation and reactions with acids. Reactions of epoxides with alcohols, ammonia derivatives and $LiAlH_4$
Carbonyl compounds: Structure, reactivity and preparation; Nucleophilic additions, Nucleophilic addition-elimination reactions with ammonia derivatives with mechanism; Mechanisms of Aldol and Benzoin condensation, Knoevenagel condensation, Claisen-Schmidt, Perkin, Cannizzaro and Wittig reaction, Beckmann and Benzil-Benzilic acid rearrangements, haloform reaction and Baeyer Villiger oxidation, α-substitution reactions, oxidations and reductions (Clemmensen, Wolff-Kishner, $LiAlH_4$, $NaBH_4$, MPV, PDC and PGC);Addition reactions of unsaturated carbonyl compounds: Michael addition. Active methylene compounds: Keto-enol tautomerism. Preparation and synthetic applications of diethyl malonate and ethyl acetoacetate.

UNIT III: CARBOXYLIC ACIDS AND THEIR DERIVATIVES [15 Hours]

Preparation, physical properties and reactions of monocarboxylic acids: Typical reactions of dicarboxylic acids, hydroxy acids and unsaturated acids: succinic/phthalic, lactic, malic, tartaric, citric, maleic and fumaric acids; Preparation and reactions of acid chlorides, anhydrides, esters and amides; Comparative study of nucleophilic sustitution at acyl group -Mechanism of acidic and alkaline hydrolysis of esters, Claisen condensation, Dieckmann and Reformatsky reactions, Hofmannbromamide degradation and Curtius rearrangement.

Sulphur containing compounds:

Preparation and reactions of thiols, thioethers and sulphonic acids.

UNIT IV: NITROGEN CONTAINING FUNCTIONAL GROUPS [15 Hours]

Preparation and important reactions of nitro and compounds, nitriles and isonitriles
Amines: Effect of substituent and solvent on basicity; Preparation and properties: Gabrielphthalimide synthesis, Carbylamine reaction, Mannich reaction, Hoffmann's exhaustive methylation, Hofmann-elimination reaction; Distinction between 1°, 2°and 3°amines with Hinsberg reagent and nitrous acid.
Diazonium Salts: Preparation and their synthetic applications.

Suggested Readings

1. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt.Ltd. (Pearson Education).
2. Finar, I. L. *Organic Chemistry* (*Volume 1*), Dorling Kindersley (India) Pvt. Ltd.=(Pearson Education).
3. Graham Solomons, T.W. *Organic Chemistry*, John Wiley & Sons, Inc. McMurry, J.E. *Fundamentals of Organic Chemistry*, 7th Ed. Cengage Learning India Edition, 2013.

Core Paper

SEMESTER III
ORGANIC CHEMISTRY II
PAPER CODE: BCH-CC7 PR
TITLE: HALOGEN, OXYGEN AND NITROGEN CONTAINING FUNCTIONAL GROUPS

TOTAL HOURS: 60 **CREDITS: 02**

Organic preparations:

i. Acetylation of one of the following compounds: amines (aniline, *o*-, *m*-, *p*toluidinesand *o*-, *m*-, *p*-anisidine) and phenols (β-naphthol, vanillin, salicylic acid) by any one method:
   a. Using conventional method.
   b. Using green approach
ii. Benzolyation of one of the following amines (aniline, *o*-, *m*-, *p*- toluidines and *o*-,*m*-, *p*-anisidine) and one of the following phenols (β-naphthol, resorcinol, pcresol)by Schotten-Baumann reaction.
iii. Oxidation of ethanol/ isopropanol (Iodoform reaction).
iv. Bromination of any one of the following:
   a. Acetanilide by conventional methods
   b. Acetanilide using green approach (Bromate-bromide method)
v. Nitration of any one of the following:
   a. Acetanilide/nitrobenzene by conventional method
   b. Salicylic acid by green approach (using ceric ammonium nitrate).
vi. Selective reduction of *meta* dinitrobenzene to *m*-nitroaniline.
vii. Reduction of *p*-nitrobenzaldehyde by sodium borohydride.
viii. Hydrolysis of amides and esters.
ix. Semicarbazone of any one of the following compounds: acetone, ethyl methylketone, cyclohexanone, benzaldehyde.
x. *S*-Benzylisothiouronium salt of one each of water soluble and water insoluble acids(benzoic acid, oxalic acid, phenyl acetic acid and phthalic acid).
xi. Aldol condensation using either conventional or green method.
xii. Benzil-Benzilic acid rearrangement.

The compounds prepared may be used for recrystallization, melting point and TLC.

Reference Books

- Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009)
- Furniss, B.S., Hannaford, A.J., Smith, P.W.G. & Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.* Pearson (2012)
- Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry:Preparation and Quantitative Analysis,* University Press (2000).

Teaching Learning Process:

- Lectures in classrooms
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Assessment Methods:

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Keywords: Functional groups, Halogens, Oxygen, Nitrogen