WEST BENGAL STATE UNIVERSITY

SYLLABUS IN CHEMISTRY (HONOURS)

PHYSICAL CHEMISTRY PORTION

UNDER CBCS

SEMESTER 1, 3 AND 5

(This is the modified syllabus only for the academic session 2020-21 for the above-mentioned semesters in view of the COVID pandemic as per resolution taken in the UGBOS meetings of the Department of Chemistry)

This document contains a total of 12 pages

***CEMACOR02T:* PHYSICAL CHEMISTRY-I**

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures **Marks: 50**

Kinetic Theory and Gaseous state
(20 Lectures) **Marks: 16**

Kinetic Theory of gases: Concept of pressure and temperature; Collision of gas molecules; Collision diameter; Collision number and mean free path; Frequency of binary collisions (similar and different molecules); ~~Rate of collision on wall and rate of effusion.~~

Maxwell's distribution of speed and energy: Nature of distribution of velocities, Maxwell's distribution of speeds in one, two and three dimensions; Kinetic energy distribution in one, two and three dimensions, calculations of average, root mean square and most probable values in each case; ~~Calculation of number of molecules having energy ≥ ε;~~ Principle of equipartition of energy and its application to calculate the classical limit of molar heat capacity of gases

Real gas and virial equation: Deviation of gases from ideal behavior; compressibility factor; Boyle temperature; Andrew's and Amagat's plots; van der Waals equation and its features; its derivation and application in explaining real gas behaviour, ~~other equations of state (Berthelot, Dietrici);~~ Existence of critical state, Critical constants in terms of van der Waals constants; Law of corresponding states; ~~virial equation of state; van der Waals equation expressed in virial form and significance of second virial coefficient; Intermolecular forces (Debye, Keesom and London interactions; LennardJones potential - elementary idea)~~

Chemical Thermodynamics
(25 Lectures) **Marks: 20**

Zeroth and 1st law of Thermodynamics: Intensive and extensive variables; state and path functions; isolated, closed and open systems; zeroth law of thermodynamics;Concept of heat, work, internal energy and statement of first law; enthalpy, *H*; relation between heat capacities, calculations of *q*, *w*, *U* and *H* for reversible, irreversible and free expansion of gases (ideal ~~and van der Waals)~~ under isothermal and adiabatic conditions; Joule's experiment and its consequence

Thermochemistry:Standard states; Heats of reaction; enthalpy of formation of molecules and ions and enthalpy of combustion and its applications; Laws of thermochemistry; bond energy, bond dissociation energy and resonance energy from thermochemical data, Kirchhoff's equations and effect of pressure on enthalpy of reactions; ~~Adiabatic flame temperature; explosion temperature~~

Second Law:Need for a Second law; statement of the second law of thermodynamics; Concept of heat reservoirs and heat engines; Carnot cycle; Physical concept of Entropy; Carnot engine and refrigerator; Kelvin – Planck and Clausius statements and equivalence of the two statements with entropic formulation; Carnot's theorem; Values of $\oint dQ/T$ and Clausius inequality; Entropy change of systems and surroundings for various processes and transformations; Entropy and unavailable work; ~~Auxiliary state functions (G and A) and their variation with T, P and V. Criteria for spontaneity and equilibrium.~~

~~Thermodynamic relations: Maxwell's relations; Gibbs- Helmholtz equation, JouleThomson experiment and its consequences; inversion temperature; Joule-Thomson coefficient for a van der Waals gas; General heat capacity relations~~

Chemical kinetics

(15 Lectures) **Marks: 14**

Rate law, order and molecularity: Introduction of rate law, Extent of reaction; rate constants, order; Forms of rates of First, second and n-th order reactions; Pseudo first order reactions (example using acid catalyzed hydrolysis of methyl acetate); Determination of order of a reaction by half-life and differential method; Opposing reactions, parallel reactions ~~and consecutive reactions (with explanation of kinetic and thermodynamic control of products; all steps first order) ; Rate equation for the fast reaction~~

Role of T and theories of reaction rate: Temperature dependence of rate constant; Arrhenius equation, energy of activation; Rate-determining step and steady-state approximation – explanation with suitable examples; Collision theory; Lindemann theory of unimolecular reaction; ~~outline of Transition State theory (classical treatment)~~

Homogeneous catalysis: Homogeneous catalysis with reference to acid-base catalysis; ~~Primary kinetic salt effect; Enzyme catalysis; Michaelis-Menten equation, LineweaverBurk plot, turn-over number~~

~~Autocatalysis; periodic reactions~~

Reference Books

1. Atkins, P. W. & Paula, J. de *Atkins' Physical Chemistry*, Oxford University Press
2. Castellan, G. W. *Physical Chemistry*, Narosa
3. McQuarrie, D. A. & Simons, J. D. *Physical Chemistry: A Molecular Approach*, Viva Press
4. Engel, T. & Reid, P. *Physical Chemistry*, Pearson
5. Levine, I. N. *Physical Chemistry*, Tata McGraw-Hill
6. Maron, S. & Prutton *Physical Chemistry*
7. Ball, D. W. *Physical Chemistry*, Thomson Press
8. Mortimer, R. G. *Physical Chemistry*, Elsevier
9. Laidler, K. J. *Chemical Kinetics*, Pearson
10. Glasstone, S. & Lewis, G.N. *Elements of Physical Chemistry*
11. Rakshit, P.C., *Physical Chemistry* Sarat Book House

12. Zemansky, M. W. & Dittman, R.H. *Heat and Thermodynamics*, Tata-McGraw-Hill
13. Rastogi, R. P. & Misra, R.R. *An Introduction to Chemical Thermodynamics*, Vikas
14. Klotz, I. M. & Rosenberg, R. M. Chemical Thermodynamics, Wiley

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CEMACOR02T: **PHYSICAL CHEMISTRY-I LAB**

(60 Lectures/Contact Hours**)** **Marks: 25**

Experiment 1: Determination of pH of unknown solution (buffer), by color matching method

~~Experiment 2: Determination of heat of neutralization of a strong acid by a strong base~~

Experiment 3: Study of kinetics of acid-catalyzed hydrolysis of methyl acetate

Experiment 4: Study of kinetics of decomposition of H_2O_2

~~Experiment 5: Determination of heat of solution of oxalic acid from solubility measurement~~

Reference Books

1. Viswanathan, B., Raghavan, P.S. *Practical Physical Chemistry* Viva Books (2009)
2. Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson
3. Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007)
4. Palit, S.R., De, S. K. *Practical Physical Chemistry* Science Book Agency
5. *University Hand Book of Undergraduate Chemistry Experiments*, edited by Mukherjee, G. N., University of Calcutta
6. Levitt, B. P. edited *Findlay's Practical Physical Chemistry* Longman Group Ltd.
7. Gurtu, J. N., Kapoor, R., *Advanced Experimental Chemistry* S. Chand & Co. Ltd.

Reference Books

1. Vogel, A. I. *Elementary Practical Organic Chemistry*, Part 1: *Small scale Preparations*, CBS Publishers and Distributors.
2. *University Hand Book of Undergraduate Chemistry Experiments*, edited by Mukherjee, G. N. University of Calcutta, 2003.
3. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009).
4. Furniss, B.S., Hannaford, A.J., Smith, P.W.G. & Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.* Pearson (2012).
5. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press (2000).
6. *Practical Workbook Chemistry (Honours), UGBS, Chemistry*, University of Calcutta, 2015.

SEMESTER-III

CEMACOR05T: **PHYSICAL CHEMISTRY-II**

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures Marks: 50

Transport processes
(15 Lectures) Marks: 14

~~Fick's law: Flux, force, phenomenological coefficients & their inter-relationship (general form), different examples of transport properties~~

Viscosity:General features of fluid flow (streamline flow and turbulent flow); Newton's equation, viscosity coefficient; Poiseuille's equation; principle of determination of viscosity coefficient of liquids by falling sphere method; Temperature variation of viscosity of liquids and comparison with that of gases

Conductance and transport number: Ion conductance; Conductance and measurement of conductance, cell constant, specific conductance, equivalent conductance and molar conductance; Variation of specific and equivalent conductance with dilution for strong and weak electrolytes; Kohlrausch's law of independent migration of ions; Equivalent and molar conductance at infinite dilution and their determination for strong and weak

electrolytes; ~~Debye – Huckel theory of Ion atmosphere (qualitative) asymmetric effect, relaxation effect and electrophoretic effect;~~ Ostwald's dilution law; Ionic mobility; Application of conductance measurement (determination of solubility product and ionic product of water); Conductometric titrations

Transport number, Principles of ~~Hittorf's and~~ Moving-boundary method; ~~Wien effect, Debye-Falkenhagen effect, Walden's rule~~

Applications of Thermodynamics – I
(25 Lectures) Marks: 20

Partial properties and Chemical potential: Chemical potential and activity, partial molar quantities, relation between Chemical potential and Gibbs' free energy and other thermodynamic state functions; variation of Chemical potential (μ) with temperature and pressure; Gibbs-Duhem equation; fugacity and fugacity coefficient; Variation of thermodynamic functions for systems with variable composition; Equations of states for these systems, Change in G, S, H and V during mixing for binary solutions

Chemical Equilibrium: Thermodynamic conditions for equilibrium, degree of advancement; van't Hoff's reaction isotherm (deduction from chemical potential); Variation of free energy with degree of advancement; Equilibrium constant and standard Gibbs' free energy change; Definitions of K_P, K_C and K_X; van't Hoff's reaction isobar and isochore from different standard states; Shifting of equilibrium due to change in external parameters e.g. temperature and pressure; variation of equilibrium constant with addition to inert gas; Le Chatelier's principle and its derivation

~~Nernst's distribution law; Application- (finding out K_{eq} using Nernst dist law for $KI+I_2 = KI_3$ and dimerization of benzene)~~

Chemical potential and other properties of ideal substances- pure and mixtures: a) Pure ideal gas-its Chemical potential and other thermodynamic functions and their changes during a change of Thermodynamic parameters of mixing; Chemical potential of an ideal gas in an ideal gas mixture; Concept of standard states and choice of standard states of ideal gases

~~b) Condensed Phase – Chemical potential of pure solid and pure liquids, Ideal solution – Definition, Raoult's law; Mixing properties of ideal solutions, chemical potential of a component in an ideal solution; Choice of standard states of solids and liquids~~

Foundation of Quantum Mechanics
(20 Lectures) Marks: 16

Beginning of Quantum Mechanics: Black-body radiation and Planck's theory of radiation; Light as particles: photoelectric ~~and Compton~~ effects; electrons as waves; Wave-particle duality: de Broglie hypothesis, Uncertainty relations (without proof)

Wave function: Schrödinger time-independent equation; nature of the equation, acceptability conditions imposed on the wave functions and probability interpretations of wave function; Orthogonal and normal functions; ~~Schmidt's orthogonalization~~

Concept of Operators: Elementary concepts of operators, eigenfunctions and eigenvalues; Linear operators; Commutation of operators, commutator and uncertainty relation; Expectation value; Hermitian operator; Postulates of Quantum Mechanics; General structure of Schrodinger equation (S.E.) ~~and time dependency;~~ Stationary state

Particle in a box: Setting up of S.E. for one-dimensional well and its solution; Comparison with free particle eigenfunctions and eigenvalues. Properties of PB wave functions (normalisation, orthogonality, probability distribution); Expectation values of x, x^2, p_x and p_x^2 and their significance in relation to the uncertainty principle; Extension of the problem to two and three dimensions and the concept of degenerate energy levels; Accidental degeneracy

~~Simple Harmonic Oscillator: setting up of the Schrodinger stationary equation, energy expression (without derivation), expression of wave function for n = 0 and n = 1 (without derivation) and their characteristic features~~

Reference Books

1. Atkins, P. W. & Paula, J. de *Atkins', Physical Chemistry*, Oxford University Press
2. Castellan, G. W. *Physical Chemistry*, Narosa
3. McQuarrie, D. A. & Simons, J. D. *Physical Chemistry: A Molecular Approach*, Viva Press
4. Levine, I. N. *Physical Chemistry*, Tata McGraw-Hill
5. Rakshit, P.C., *Physical Chemistry*, Sarat Book House
6. Moore, W. J. *Physical Chemistry*, Orient Longman
7. Mortimer, R. G. *Physical Chemistry*, Elsevier
8. Denbigh, K. *The Principles of Chemical Equilibrium* Cambridge University Press
9. Engel, T. & Reid, P. *Physical Chemistry*, Pearson
10. Levine, I. N. *Quantum Chemistry*, PHI
11. Atkins, P. W. *Molecular Quantum Mechanics*, Oxford
12. Zemansky, M. W. & Dittman, R.H. *Heat and Thermodynamics*, Tata-McGraw-Hill
13. Rastogi, R. P. & Misra, R.R. *An Introduction to Chemical Thermodynamics*, Vikas
14. Klotz, I.M., Rosenberg, R. M. *Chemical Thermodynamics:Basic Concepts and Methods* Wiley
15. Glasstone, S. *An Introduction to Electrochemistry*, East-West Press

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CEMACOR05P: **PHYSICAL CHEMISTRY-II LAB**

60 (Lectures/Contact Hours) Marks: 25

Experiment 1: Study of viscosity of unknown liquid (glycerol, sugar) with respect to water

~~Experiment 2: Determination of partition coefficient for the distribution of I_2 between water and CCl_4~~

~~Experiment 3: Determination of K_{eq} for $KI + I_2 = KI_3$, using partition coefficient between water and CCl_4~~

Experiment 4: Conductometric titration of an acid (strong, weak/ monobasic, dibasic) against base strong

~~Experiment 5: Study of saponification reaction conductometrically~~

Experiment 6: Verification of Ostwald's dilution law and determination of K_a of weak acid

Reference Books

1. Viswanathan, B., Raghavan, P.S. *Practical Physical Chemistry* Viva Books (2009)
2. Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson
3. Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007)
4. Palit, S.R., De, S. K. *Practical Physical Chemistry* Science Book Agency
5. *University Hand Book of Undergraduate Chemistry Experiments*, edited by Mukherjee, G. N., University of Calcutta
6. Levitt, B. P. edited *Findlay's Practical Physical Chemistry* Longman Group Ltd.
7. Gurtu, J. N., Kapoor, R., *Advanced Experimental Chemistry* S. Chand & Co. Ltd.

CEMACOR06T: **INORGANIC CHEMISTRY-II**

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures Marks: 50

Chemical Bonding-I
(24 Lectures) Marks: 20

(i) *Ionic bond:* General characteristics, types of ions, size effects, radius ratio rule and its application and limitations. Packing of ions in crystals. Born-Landé equation with derivation and importance of Kapustinskii expression for lattice energy. Madelung constant, Born-Haber cycle and its application, Solvation energy. Defects in solids (elememtary idea). Solubility energetics of dissolution process.

(ii) *Covalent bond:* Polarizing power and polarizability, ionic potential,Fazan's rules. Lewis structures, formal charge. Valence Bond Theory. The hydrogen molecule (Heitler-London approach), directional character of covalent bonds, hybridizations, equivalent and non-equivalent hybrid orbitals, Bent's rule, Dipole moments, VSEPR theory, shapes of

13. Levine, I. N. Quantum Chemistry, PHI
14. Atkins, P. W. Molecular Quantum Mechanics, Oxford

CEMACOR14P: **PHYSICAL CHEMISTRY- IV LAB**

(60 Lectures/Contact Hours) Marks: 25

Experiment 1: Determination of surface tension of a liquid using Stalagmometer

Experiment 2: Determination of CMC from surface tension measurements

Experiment 3: Verification of Beer and Lambert's Law for $KMnO_4$ and $K_2Cr_2O_7$ solution

Experiment 4: Study of kinetics of $K_2S_2O_8$ + KI reaction, spectrophotometrically

Experiment 5: Determination of pH of unknown buffer, spectrophotometrically

Experiment 6: Spectrophotometric determination of CMC

Reference Books

1. Viswanathan, B., Raghavan, P.S. *Practical Physical Chemistry* Viva Books (2009)
2. Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson
3. Harris, D. C. *Quantitative Chemical Analysis*, 6th Ed., Freeman (2007)
4. Palit, S.R., De, S. K. *Practical Physical Chemistry* Science Book Agency
5. *University Hand Book of Undergraduate Chemistry Experiments*, edited by Mukherjee, G. N., University of Calcutta
6. Levitt, B. P. edited *Findlay's Practical Physical Chemistry* Longman Group Ltd.
7. Gurtu, J. N., Kapoor, R., *Advanced Experimental Chemistry* S. Chand & Co. Ltd.

DISCIPLINE SPECIFIC ELECTIVE COURSE (HONOURS) IN CHEMISTRY

CEMADSE01T:
ADVANCED PHYSICAL CHEMISTRY (Credits: Theory-04, Practicals-02)

Theory
(60 Lecturers)
Crystal Structure
(20 Lectures) Marks: 18

Bravais Lattice and Laws of Crystallography: Types of solid, Bragg's law of diffraction; Laws of crystallography; Permissible symmetry axes in crystals; Lattice, space lattice, unit cell, crystal planes, Bravais lattice. ~~Packing of uniform hard sphere, close packed arrangements (fcc and hcp); Tetrahedral and octahedral voids.~~ Void space in ~~p-type, F-type and I-type~~ cubic systems

Crystal planes: Distance between consecutive planes [cubic, ~~tetragonal and orthorhombic lattices~~]; Indexing of planes, Miller indices; calculation of d_{hkl}; Relation between molar mass and unit cell dimension for cubic system; ~~Laue's diffraction;~~ Bragg's law (derivation)

~~Determination of crystal structure: Powder method;~~ Structure of NaCl and KCl crystals

Statistical Thermodynamics
(20 Lectures) Marks: 16

Configuration: Macrostates, microstates and configuration; ~~calculation of microstates with harmonic oscillator and~~ tossing of coins; variation of W with E; equilibrium configuration

Boltzmann distribution: Thermodynamic probability, entropy and probability, Boltzmann distribution formula (with derivation); Applications to barometric distribution; ~~Concept of ensemble - canonical ensemble and grand canonical ensembles~~

Partition function: molecular partition function and thermodynamic properties (U, H, S, C_V, q, P); Partition function correlating ~~– Chemical equilibrium and Maxwell's speed distribution; Gibbs' paradox;~~ Ideal gas equation

Special selected topics
(20 Lectures) Marks: 16

Specific heat of solid: ~~Coefficient of thermal expansion, thermal compressibility of solids;~~ Dulong –Petit's law; Perfect Crystal model, Einstein's theory ~~– derivation from partition function,~~ limitations; Debye's T^3 law – analysis at the two extremes

3rd law: Absolute entropy, Plank's law, Calculation of entropy, Nernst heat theorem
Adiabatic demagnetization: Approach to zero Kelvin, adiabatic cooling, demagnetization, adiabatic demagnetization – involved curves

Polymers: Classification of polymers, nomenclature, Molecular forces and chemical bonding in polymers, ~~Texture of Polymers;~~ Criteria for synthetic polymer formation; Relationships between functionality, extent of reaction and degree of polymerization; Mechanism and kinetics of step growth and copolymerization; Conducting polymers

Reference Books

1. Castellan, G. W. *Physical Chemistry*, Narosa
2. Levine, I. N. *Physical Chemistry*, Tata McGraw-Hill
3. Moore, W. J. *Physical Chemistry*, Orient Longman
4. Atkins, P. W. & Paula, J. de *Atkins', Physical Chemistry*, Oxford University Press
5. McQuarrie, D. A. & Simons, J. D. *Physical Chemistry*: A Molecular Approach, Viva Press
6. Engel, T. & Reid, P. *Physical Chemistry*, Pearson
7. Nash, L. K. *Elements of Statistical Thermodynamics*, Dover
8. Rastogi, R. P. & Misra, R.R. *An Introduction to Chemical Thermodynamics*, Vikas
9. Zemansky, M. W. & Dittman, R.H. *Heat and Thermodynamics*, Tata-McGraw-Hill
10. Billmeyer, F. W. *Textbook of Polymer Science*, John Wiley & Sons, Inc.
11. Seymour, R. B. & Carraher, C. E. *Polymer Chemistry: An Introduction*, Marcel Dekker, Inc.
12. Odian, G. *Principles of Polymerization*, Wiley
13. Billmeyer, F. W. *Textbook of Polymer Science*, Wiley Interscience, 1971.

CEMADSE01P: **ADVANCED PHYSICAL CHEMISTRY LAB**

(60 Lectures/Contact Hours) Marks: 25

Computer programs based on numerical methods for

Programming 1: Roots of equations: (e.g. volume of van der Waals gas and comparison with ideal gas, pH of a weak acid)

Programming 2: Numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations)

Programming 3: Numerical integration (e.g. entropy/ enthalpy change from heat capacity data), probability distributions (gas kinetic theory) and mean values

Programming 4: Matrix operations (Application of Gauss-Siedel method in colourimetry)

Programming 5: Simple exercises using molecular visualization software

Reference Books

1. McQuarrie, D. A. *Mathematics for Physical Chemistry* University Science Books (2008)
2. Mortimer, R. *Mathematics for Physical Chemistry*. 3rd Ed. Elsevier (2005)
3. Yates, P. *Chemical Calculations*. 2nd Ed. CRC Press (2007)
4. Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007) Chapters 3-5
5. Noggle, J. H. *Physical Chemistry on a Microcomputer*. Little Brown & Co. (1985)

CEMADSE02T: **ANALYTICAL METHODS IN CHEMISTRY**
(Credits: Theory-04, Practicals-02)
Theory: 60 Lectures Marks: 50

Qualitative and quantitative aspects of analysis:
(05 Lectures) Marks: 06

Sampling, evaluation of analytical data, errors, accuracy and precision, methods of their expression, normal law of distribution if indeterminate errors, statistical test of data; F, Q and t test, rejection of data, and confidence intervals.

Optical methods of analysis:
(25 Lectures) Marks: 16

Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules, validity of Beer-Lambert's law.

UV-Visible Spectrometry: Basic principles of instrumentation (choice of source,monochromator and detector) for single and double beam instrument;
Basic principles of quantitative analysis: estimation of metal ions from aqueous solution,geometrical isomers, keto-enol tautomers. Determination of composition of metal complexes using Job's method of continuous variation and mole ratio method. *Infrared Spectrometry:* Basic principles of instrumentation (choice of source, monochromator& detector) for single and double beam instrument; sampling techniques.

Structural illustration through interpretation of data, Effect and importance of isotope substitution.

Flame Atomic Absorption and Emission Spectrometry: Basic principles of instrumentation(choice of source, monochromator, detector, choice of flame and Burner designs. Techniques of atomization and sample introduction; Method of background