



List of New Course(s) Introduced

Department : Chemistry

Programme Name : B.Sc.

Academic Year : 2018-19

List of New Course(s) Introduced

Sr. No.	Course Code	Name of the Course
01.	CBT-1	Inorganic Chemistry I
02.	CBL-1	Inorganic Chemistry I Practical
03.	CBT-2	Physical Chemistry I
04.	CBL-2	Physical Chemistry I Practical
05.	GE-1	Generic Elective – 1
06.	GE-1 LAB	Generic Elective Practical – 1
07.	CBT-3	Organic Chemistry I
08.	CBL-3	Organic Chemistry I Practical
09.	CBT-4	Physical Chemistry II
10.	CBL-4	Physical Chemistry II Practical
11.	GE-2	Generic Elective – 2
12.	GE-2 LAB	Generic Elective Practical – 2



Minutes of Meetings (MoM) of Board of Studies (BoS)

Academic Year : 2018-19

School : School of Studies of Physical Science

Department : Chemistry

Date and Time : Nov. 03, 2017 - 11:30 AM

Venue : Meeting room

The scheduled meeting of member of Board of Studies (BoS) of Department of Chemistry, School of Studies of Physical Science, Guru Ghasidas Vishwavidyalaya, Bilaspur was held to design and discuss the structure and scheme of examination of Integrated UG/PG, M. Sc. Chemistry syllabi.

The following members were present in the meeting:

1. Prof. Bali Ram (External Expert Member BoS, Dept. of Chemistry, BHU, Varanasi)
2. Prof. G. K. Patra (Member BoS, Dept. of Chemistry)
3. Dr. Charu Arora (HOD, Associate Prof., Dept. of Chemistry-cum Chairman, BOS)
4. Dr. Arti Srivastava (Member BoS, Assistant Professor, Dept. of Chemistry)

Following points were discussed during the meeting

1. Draft prepared to revise course structure and scheme of examination in the light of UGC directives (as per CBCS Scheme) to be implemented from 2018-19.
2. Elective paper Advanced Quantum and Computational Chemistry (CMT-405) has been incorporated in M.Sc. IV sem.
3. The core paper Organic Chemistry-IV (CBT-503) of B.Sc.-Vth sem has been interchanged with core paper Physical Chemistry-IV (CBT-601) to justify semester wise teaching load.

The following new courses were introduced in the B. Sc. and M. Sc.:

- ❖ B. Sc. CBCS scheme
 - Inorganic Chemistry I (CBT-1)
 - Inorganic Chemistry I Practical (CBL-1)
 - Physical Chemistry I (CBT-2)
 - Physical Chemistry I Practical (CBL-2)
 - Generic Elective - I (GE-1)
 - Generic Elective Practical - I (GE-1 LAB)
 - Organic Chemistry I (CBT-3)
 - Organic Chemistry I Practical (CBL-3)
 - Physical Chemistry II (CBT-4)
 - Physical Chemistry II Practical (CBL-4)
 - Generic Elective - 2 (GE-2)
 - Generic Elective Practical - 2 (GE-2 Lab)

गुरु घासीदास विश्वविद्यालय
(केन्द्रीय विश्वविद्यालय अधिनियम 2009 क्र. 25 के अंतर्गत स्थापित केन्द्रीय विश्वविद्यालय)
कोनी, बिलासपुर - 495009 (छ.ग.)



Guru Ghasidas Vishwavidyalaya
(A Central University Established by the Central Universities Act 2009 No. 25 of 2009)
Koni, Bilaspur - 495009 (C.G.)

❖ Advanced Quantum and Computational Chemistry (CMT-405)

शासक/Head
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Scheme and Syllabus

B.Sc. Hon's Programme: Department of Chemistry

Semester	Course Opted	Course Code	Name of the course	Credit	Hour / week
I	Core-1	CBT-1	Inorganic Chemistry-I:	4	4
	Core -1 Practical	CBL-1	Inorganic Chemistry-1 Practical	2	4
	Core -2	CBT-2	Physical Chemistry I:	4	4
	Core -2 Practical	CBL-2	Physical Chemistry-I Practical	2	4
	Generic Elective -1		1A Physics-I 1B Mathematics-I 1C Zoology-I 1D Botany-I	4	4
	Generic Elective - Practical		Generic Elective – Practical-I	2	4
	Ability Enhancement Compulsory Course (AECC)		English Communication / MIL	4	4
	ECA		ECA-Extracurricular activity/ Tour, Field visit/ Industrial training/ NSS/ Swachhta/ vocational Training/ Sports/ others	2	(2)
			TOTAL	24	28
	II	Core-3	CBT-3	Organic Chemistry-I	4
Core -3 Practical		CBL-3	Organic Chemistry-I Practical	2	4
Core -4		CBT-4	Physical Chemistry-II	4	4
Core -4 Practical		CBL-4	Physical Chemistry-II Practical	2	4
Generic Elective -2			2A Physics-II 2B Mathematics-II 2C Zoology-II 2D Botany-II	4	4
Generic Elective - Practical			Generic Elective – Practical-II	2	4
Ability Enhancement Compulsory Course (AECC)			Environmental Science	4	4
ECA			ECA-Extracurricular activity/ Tour, Field visit/ Industrial training/ NSS/ Swachhta/ vocational Training/ Sports/ others	2	(2)
			Total	24	28

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CORE COURSE (HONOURS IN CHEMISTRY)

Semester I

CHEMISTRY-C I: INORGANIC CHEMISTRY-I (CBT-1)

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Atomic Structure:

Bohr's theory, its limitations and atomic spectrum of hydrogen atom. Wave mechanics; de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Schrödinger's wave equation, significance of ψ and ψ^2 . Quantum numbers and their significance. Normalized and orthogonal wave functions. Sign of wave functions. Radial and angular wave functions for hydrogen atom. Radial and angular distribution curves. Shapes of s , p , d and f orbitals. Contour boundary and probability diagrams.

Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, Aufbau's principle and its limitations, Variation of orbital energy with atomic number.

Periodicity of Elements:

s , p , d , f block elements, the long form of periodic table. Detailed discussion of the following properties of the elements, with reference to s & p -block.

(a) Effective nuclear charge, shielding or screening effect, Slater rules, variation of effective nuclear charge in periodic table.

(b) Atomic radii (van der Waals)

(c) Ionic and crystal radii.

(d) Covalent radii (octahedral and tetrahedral)

(e) Ionization enthalpy, Successive ionization enthalpies and factors affecting ionization energy. Applications of ionization enthalpy.

(f) Electron gain enthalpy, trends of electron gain enthalpy.

(g) Electronegativity, Pauling's/ Mulliken's/ Allred Rachow's/ and Mulliken-Jaffe's electronegativity scales. Variation of electronegativity with bond order, partial charge, hybridization, group electronegativity. Sanderson's electron density ratio.



Chemical Bonding:

(i) *Ionic bond*: General characteristics, types of ions, size effects, radius ratio rule and its 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.

(ii) *Covalent bond*: Lewis structure, Valence Bond theory (Heitler-London approach). Energetics of hybridization, equivalent and non-equivalent hybrid orbitals. Bent's rule, Resonance and resonance energy, Molecular orbital theory. Molecular orbital diagrams of diatomic and simple polyatomic molecules N_2 , O_2 , C_2 , B_2 , F_2 , CO , NO , and their ions; HCl , BeF_2 , CO_2 , (idea of s-p mixing and orbital interaction to be given). Formal charge, Valence shell electron pair repulsion theory (VSEPR), shapes of simple molecules and ions containing lone pairs and bond pairs of electrons, multiple bonding (σ and π bond approach) and bond lengths.

Covalent character in ionic compounds, polarizing power and polarizability. Fajan's rules and consequences of polarization.

Ionic character in covalent compounds: Bond moment and dipole moment. Percentage ionic character from dipole moment and electronegativity difference.

(iii) *Metallic Bond*: Qualitative idea of valence bond and band theories. Semiconductors and insulators, defects in solids.

(iv) *Weak Chemical Forces*: van der Waals forces, ion-dipole forces, dipole-dipole interactions, induced dipole interactions, Instantaneous dipole-induced dipole interactions. Repulsive forces, Hydrogen bonding (theories of hydrogen bonding, valence bond treatment) Effects of chemical force, melting and boiling points, solubility energetics of dissolution process.

Oxidation-Reduction:

Redox equations, Standard Electrode Potential and its application to inorganic reactions.

Principles involved in volumetric analysis to be carried out in class.

(4 Lectures)

Reference Books:

- Lee, J.D. Concise Inorganic Chemistry, ELBS, 1991.
- Douglas, B.E. and Mc Daniel, D.H., Concepts & Models of Inorganic Chemistry, Oxford, 1970
- Atkins, P.W. & Paula, J. Physical Chemistry, Oxford Press, 2006.
- Day, M.C. and Selbin, J. Theoretical Inorganic Chemistry, ACS Publications 1962.

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CHEMISTRY LAB-C1: INORGANIC CHEMISTRY-1 PRACTICAL (CBL-1)
60 LECTURES

(A) Titrimetric Analysis

- (i) Calibration and use of apparatus
- (ii) Preparation of solutions of different Molarity/Normality of titrants

(B) Acid-Base Titrations

- (i) Estimation of carbonate and hydroxide present together in mixture.
- (ii) Estimation of carbonate and bicarbonate present together in a mixture.
- (iii) Estimation of free alkali present in different soaps/detergents

(C) Oxidation-Reduction Titrimetry

- (i) Estimation of Fe(II) and oxalic acid using standardized KMnO_4 solution.
- (ii) Estimation of oxalic acid and sodium oxalate in a given mixture.
- (iii) Estimation of Fe(II) with $\text{K}_2\text{Cr}_2\text{O}_7$ using internal (diphenylamine, anthranilic acid) and external indicator.

Reference text:

- 1. Vogel, A.I. A Textbook of Quantitative Inorganic Analysis, ELBS.

CHEMISTRY -C II: PHYSICAL CHEMISTRY I (CBT-2)

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Gaseous state:

Kinetic molecular model of a gas: postulates and derivation of the kinetic gas equation; collision frequency; collision diameter; mean free path and viscosity of gases, including their temperature and pressure dependence, relation between mean free path and coefficient of viscosity, calculation of σ from η ; variation of viscosity with temperature and pressure.

Maxwell distribution and its use in evaluating molecular velocities (average, root mean square and most probable) and average kinetic energy, law of equipartition of energy, degrees of freedom and molecular basis of heat capacities.

Behaviour of real gases: Deviations from ideal gas behaviour, compressibility factor, Z , and its variation with pressure for different gases. Causes of deviation from ideal behaviour. van



der Waals equation of state, its derivation and application in explaining real gas behaviour, mention of other equations of state (Berthelot, Dietrici); virial equation of state; van der Waals equation expressed in virial form and calculation of Boyle temperature. Isotherms of real gases and their comparison with van der Waals isotherms, continuity of states, critical state, relation between critical constants and van der Waals constants, law of corresponding states.

Liquid state:

Qualitative treatment of the structure of the liquid state; Radial distribution function; physical properties of liquids; vapour pressure, surface tension and coefficient of viscosity, and their determination. Effect of addition of various solutes on surface tension and viscosity. Explanation of cleansing action of detergents. Temperature variation of viscosity of liquids and comparison with that of gases.

Qualitative discussion of structure of water.

Solid state:

Nature of the solid state, law of constancy of interfacial angles, law of rational indices, Miller indices, elementary ideas of symmetry, symmetry elements and symmetry operations, qualitative idea of point and space groups, seven crystal systems and fourteen Bravais lattices; X-ray diffraction, Bragg's law, a simple account of rotating crystal method and powder pattern method. Analysis of powder diffraction patterns of NaCl, CsCl and KCl. Defects in crystals. Glasses and liquid crystals.

Ionic equilibria:

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect; dissociation constants of mono-, di- and triprotic acids (exact treatment).

Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions; derivation of Henderson equation and its applications; buffer capacity, buffer range, buffer action and applications of buffers in analytical chemistry and biochemical processes in the human body.

Solubility and solubility product of sparingly soluble salts – applications of solubility product principle. Qualitative treatment of acid – base titration curves (calculation of pH at various stages). Theory of acid–base indicators; selection of indicators and their limitations.

Multistage equilibria in polyelectrolyte systems; hydrolysis and hydrolysis constants.

Reference Books:

- Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry Ed., Oxford University Press (2006).
- Ball, D. W. Physical Chemistry Thomson Press, India (2007).
- Castellan, G. W. Physical Chemistry 4th Ed. Narosa (2004).
- Mortimer, R. G. Physical Chemistry 3rd Ed. Elsevier: NOIDA, UP (2009).



CHEMISTRY LAB-C II: PHYSICAL CHEMISTRY-1 PRACTICAL (CBL-2)
60 LECTURES

1. **Surface tension measurements.**
 - a. Determine the surface tension by (i) drop number (ii) drop weight method.
 - b. Study the variation of surface tension of detergent solutions with concentration.
2. **Viscosity measurement using Ostwald's viscometer.**
 - a. Determination of viscosity of aqueous solutions of (i) polymer (ii) ethanol and (iii) sugar at room temperature.
 - b. Study the variation of viscosity of sucrose solution with the concentration of solute.
3. **Indexing of a given powder diffraction pattern of a cubic crystalline system.**
4. **pH metry**
 - a. Study the effect on pH of addition of HCl/NaOH to solutions of acetic acid, sodium acetate and their mixtures.
 - b. Preparation of buffer solutions of different pH
 - i. Sodium acetate-acetic acid
 - ii. Ammonium chloride-ammonium hydroxide
 - c. pH metric titration of (i) strong acid vs. strong base, (ii) weak acid vs. strong base.
 - d. Determination of dissociation constant of a weak acid.

Any other experiment carried out in the class.

Reference Books

- Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
- 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).

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Semester II

CHEMISTRY-C III: ORGANIC CHEMISTRY I (CBT-3)

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Structure and Bonding: Classification, nomenclature and general structure of organic compounds. Hybridization, orbital representation of methane, ethane, ethylene, acetylene and benzene. Bond energy, bond length and bond angles. Polarity of covalent bonds—Inductive, resonance, hyper-conjugation and steric inhibition in resonance and its influence on acidity and basicity of organic compounds.

Mechanism of Organic reactions: Curved arrow notation, drawing electron movements with arrows, half-headed and double headed arrows. Homolysis and heterolysis of carbon-carbon bonds; Reactive species e.g. Carbocations, carbanions, free radicals and their stability. Nucleophiles and electrophiles.

Alkanes and cycloalkanes: Preparation and general reactions of alkanes and cycloalkanes, Bayer Strain theory of strainless ring; Conformation of ethane, *n*-butane and cyclohexane, chlorination of methane and side chain chlorination of toluene.

Alkenes: General methods for preparation of alkenes, Reactions of alkenes: Addition reactions (Electrophilic and free radical), Halogenation, Hydrohalogenation, Hydration, Hydroxylation, Hydroboration-oxidation, Mercuration-demercuration, Epoxidation and Ozonolysis.

Dienes: Conjugated and isolated Dienes; 1,2- versus 1,4-addition. Diels-Alder reaction of dienes: Mechanism

Alkynes: Preparation of alkynes, acidity and metal acetylides, Electrophilic addition reactions viz., Halogenation, Hydrohalogenation, Hydration, Hydroboration-oxidation, Mercuration-demercuration and Ozonolysis.

Books Recommended:

1. "Organic Chemistry", R. T. Morrison and R. N. Boyd, 6th Edition (1992), Prentice-Hall of India (P)Ltd., New Delhi.
2. "Organic Chemistry", S. M. Mukherjee, S. P. Singh, and R. P. Kapoor, 1st Edition (1985), New Age International (P) Ltd. Publishers, New Delhi.
3. "Organic Chemistry", I. L. Finar, [Vol. I, 6th Edition (1973), Reprinted in 1980 & Vol. II, 5th Edition (1975), Reprinted in 1996], ELBS and Longman Ltd., New Delhi.
4. "Organic Chemistry – Structure and Reactivity", Seyhan N. Ege, 3rd Edition (1998), AITBS Publishers and Distributors, Delhi.
5. "Organic Chemistry", Paula Y. Bruice, 2nd Edition, Prentice-Hall, International Edition (1998).
6. "Organic Chemistry", G. Solomon, Willey India, Paper Back, 9th Edition.
7. "Modern Organic Chemistry", M. K. Jain and S. C. Sharma, Vishal Publishing CO. Jalandhar, India, 4th Edition (2012).



PRACTICAL CORE COURSE – III ORGANIC CHEMISTRY –I LAB (CBL-3)

60 Lectures

1. Checking the calibration of the thermometer
2. Purification of organic compounds by crystallization using the following solvents:
a. Water b. Alcohol, c. Alcohol-Water
3. Determination of the melting points of unknown organic compounds (Kjeldahl method and electrically heated melting point apparatus)
4. Effect of impurities on the melting point – mixed melting point of two unknown organic compounds.
5. Detection of special elements (N, S, Cl, Br, I).

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)

CHEMISTRY -C IV: PHYSICAL CHEMISTRY II (CBT-4)

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Chemical Thermodynamics:

Intensive and extensive variables; state and path functions; isolated, closed and open systems; zeroth law of thermodynamics.

First law: Concept of heat, q , work, w , internal energy, U , 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.

Thermochemistry: Heats of reactions: standard states; enthalpy of formation of molecules and ions and enthalpy of combustion and its applications; calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data, effect of temperature (Kirchhoff's equations) and pressure on enthalpy of reactions. Adiabatic flame temperature, explosion temperature.

Second Law: Concept of entropy; thermodynamic scale of temperature, statement of the second law of thermodynamics; molecular and statistical interpretation of entropy. Calculation of entropy change for reversible and irreversible processes.



Third Law: Statement of third law, concept of residual entropy, calculation of absolute entropy of molecules.

Free Energy Functions: Gibbs and Helmholtz energy; variation of S , G , A with T , V , P ; Free energy change and spontaneity. Relation between Joule-Thomson coefficient and other thermodynamic parameters; inversion temperature; Gibbs-Helmholtz equation; Maxwell relations; thermodynamic equation of state.

Systems of Variable Composition:

Partial molar quantities, dependence of thermodynamic parameters on composition; Gibbs-Duhem equation, chemical potential of ideal mixtures, change in thermodynamic functions in mixing of ideal gases.

Chemical Equilibrium:

Criteria of thermodynamic equilibrium, degree of advancement of reaction, chemical equilibria in ideal gases, concept of fugacity. Thermodynamic derivation of relation between Gibbs free energy of reaction and reaction quotient. Coupling of exoergic and endoergic reactions. Equilibrium constants and their quantitative dependence on temperature, pressure and concentration. Free energy of mixing and spontaneity; thermodynamic derivation of relations between the various equilibrium constants K_p , K_c and K_x . Le Chatelier principle (quantitative treatment); equilibrium between ideal gases and a pure condensed phase.

Solutions and Colligative Properties:

Dilute solutions; lowering of vapour pressure, Raoult's and Henry's Laws and their applications. Excess thermodynamic functions.

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] and amount of solute. Applications in calculating molar masses of normal, dissociated and associated solutes in solution.

Reference Books

- Peter, A. & Paula, J. de. *Physical Chemistry 9th Ed.*, Oxford University Press (2011).
- Castellan, G. W. *Physical Chemistry 4th Ed.*, Narosa (2004).
- Engel, T. & Reid, P. *Physical Chemistry 3rd Ed.*, Prentice-Hall (2012).
- McQuarrie, D. A. & Simon, J. D. *Molecular Thermodynamics* Viva Books Pvt. Ltd.: New Delhi (2004).
- Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S. *Commonly Asked Questions in Thermodynamics*. CRC Press: NY (2011).
- Levine, I. N. *Physical Chemistry 6th Ed.*, Tata Mc Graw Hill (2010).
- Metz, C. R. *2000 solved problems in chemistry*, Schaum Series (2006)



CHEMISTRY LAB- C IV PHYSICAL CHEMISTRY-II LAB (CBL-4)

60 Lectures

Thermochemistry

- (a) Determination of heat capacity of a calorimeter for different volumes using change of enthalpy data of a known system (method of back calculation of heat capacity of calorimeter from known enthalpy of solution or enthalpy of neutralization).
- (b) Determination of heat capacity of the calorimeter and enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
- (c) Calculation of the enthalpy of ionization of ethanoic acid.
- (d) Determination of heat capacity of the calorimeter and integral enthalpy (endothermic and exothermic) solution of salts.
- (e) Determination of basicity/proticity of a polyprotic acid by the thermochemical method in terms of the changes of temperatures observed in the graph of temperature versus time for different additions of a base. Also calculate the enthalpy of neutralization of the first step.
- (f) Determination of enthalpy of hydration of copper sulphate.
- (g) Study of the solubility of benzoic acid in water and determination of ΔH .

Any other experiment carried out in the class.

Reference Books

- Khosla, B. D.; Garg, V. C. & Gulati, A., *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
- Athawale, V. D. & Mathur, P. *Experimental Physical Chemistry* New Age International: New Delhi (2001).

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