UNIVERSITY OF KERALA

SYLLABUS FOR

M. Sc. PROGRAMME IN BRANCH VI
MEDICINAL CHEMISTRY

**(Revised Syllabi under Semester System
with effect from 2016 Admission)**

PREAMBLE

The syllabi of M.Sc programmes in Chemistry offered in the affiliated colleges of the University under Semester system have been revised and the revised syllabi are to be effective from 2016 admission. There are four independent PG programmes in Chemistry, namely **M.Sc**. **Programme in Branch III - Chemistry**, **M.Sc. Programme in Branch IV -Analytical Chemistry and M.Sc. Programme in Branch V - Applied Chemistry and Branch VI Medicinal Chemistry**. All these four PG programmes are equivalent in all respect for employment and higher studies. Each of these four PG programmes shall extend over a period of two academic years comprising of four semesters, each of 450 hours in 18 weeks duration. The syllabi and scheme of examinations of these four programmes are detailed below. The theory courses of the first three Semesters and the practical courses of the first two semesters of the four programmes are common, and therefore, the examinations of these four PG programmes are to be conducted with common question papers for the first three semesters by a common Board of Examiners. These syllabi are effective from 2016 admission in affiliated colleges of the university.

M.Sc. PROGRAMME IN BRANCH VI - MEDICAL CHEMISTRY

(Revised syllabus under semester system with effect from 2016 admission)

SYLLABUS AND SCHEME OF EXAMINATION

Course No. and Title	Hours per week		Duration for ESA in hours	Marks for CA	Marks for ESA	Total marks
	L	P				
SEMESTER I*						
CM 211 Inorganic Chemistry I	5		3	25	75	100
CM 212 Organic Chemistry I	5		3	25	75	100
CM 213 Physical Chemistry I	5		3	25	75	100
CM 214 Inorganic Practicals I		3	(To be continued in Semester II)			
CM 215 Organic Practicals I		3	(To be continued in Semester II)			
CM 216 Physical Practicals I		4	(To be continued in Semester II)			
			Total marks for semester 1			300
*Distribution of teaching hours/week: Theory- 15 hours, Practicals- 10 hours						
SEMESTER II*						
CM 221 Inorganic Chemistry II	5		3	25	75	100
CM 222 Organic Chemistry II	5		3	25	75	100
CM 223 Physical Chemistry II	5		3	25	75	100
CM 214 Inorganic Practicals I		3	6	25	75	100
CM 215 Organic Practicals I		3	6	25	75	100
CM 216 Physical Practicals I		4	6	25	75	100
			Total marks for Semester II			600
*Distribution of teaching hours/week: Theory- 15 hours, Practicals- 10 hours						

SEMESTER III*						
CM 231 Inorganic Chemistry III	5		3	25	75	100
CM 232 Organic Chemistry III	5		3	25	75	100
CM 233 Physical Chemistry III	5		3	25	75	100
CM 234 Quantitative Organic Practical		3	(To be continued in Semester IV)			
CM 235 Computational Techniques Lab I		3	(To be continued in Semester IV)			
CM 236 Computational Techniques Lab I		4	(To be continued in Semester IV)			
			Total marks for semester III			300

*Distribution of teaching hours/week: Theory- 15 hours, Practicals- 10 hours

SEMESTER IV*						
CM 241 Introductory Course in Medical Chemistry	5			25	75	100
CM 242 Advanced Course in Medicinal Chemistry	5			25	75	100
CM 234 Quantitative Organic Practical		3	6	25	75	100
CM 235 Computational Techniques Lab I		3	6	25	75	100
CM 236 Computational Techniques Lab I		4	6	25	75	100
CM 243(a) Dissertation	5				70	70
CM 243(b) Visit to R & D Centre					5	5
Comprehensive viva-voce					25	25
			Total marks for Semester IV			600
			Grand total (for semesters I-IV)			1800

*Distribution of teaching hours/week: Theory- 10 hours, 5 hours for discussion on project

M.Sc. PROGRAMME IN BRANCH VI- MEDICINAL CHEMISTRY

(Revised syllabus Under Semester System w.e.f. 2016 Admissions)

SEMESTER I

CM 211 INORGANIC CHEMISTRY I

Total 90 h

Unit I Coordination chemistry-I: Theories of metal complexes   **18 h**

Types of ligands and complexes. Isomerism: Structural, geometrical and optical isomerism. Crystal field theory: Splitting of d orbitals in octahedral, tetragonal, square planar, tetrahedral, trigonal bipyramidal

and square pyramidal fields. Jahn-Teller theorem, evidence for JT effect, static and dynamic JT effect. Crystal field stabilization energy (CFSE) and its calculations. Octahedral Site Stabilization Energy. Factors affecting the splitting parameter. Spectrochemical series. Evidence of covalency in Metal-Ligand bond, introduction to Ligand field theory. Molecular orbital theory. Sigma and pi bondings in complexes. MO diagrams of octahedral and tetrahedral complexes with and without pi bonds. Experimental evidence of pi bond on the stability of sigma bond. Nephelauxetic effect.

Unit II Analytical principles   18 h

Evaluation of analytical data: Accuracy and precision. Standard deviation, variance and coefficient of variation. Student 't' test, 'Q' test, and 'F' test. Confidence limits. Errors: Classification, distribution, propagation, causes and minimization of errors. Significant figures and computation rules. Correlation analysis: Scatter diagram. Correlation coefficient,r. Calculation of r by the method of least squares. Volumetric methods: Classification of reactions in volumetry. Theories of indicators. Acid-base, redox, adsorption, metallochromic indicators. Complexometric titrations: Titration using EDTA-direct and back titration methods. Precipitation titrations. Redox titrations. Titrations in non-aqueous solvents. Organic reagents used in gravimetry: Oxine, dimethylglyoxime and cupferron. Principle and instrumentation of TG, DTA and DSC. Factors affecting TG and DTA curves. Applications of TG DTA and DSC in the study of metal complexes.

Unit III Molecular symmetry   18 h

Symmetry and Character table: Symmetry elements and symmetry operation. Matrix representation of symmetry operations. Character of a matrix. Conditions for a set of elements to form a group. Point groups. Multiplication of operations. Group multiplication table. Similarity transformation and classification of symmetry operation, Matrix representation of point group. Reducible and Irreducible representations. The Great Orthogonality theorem. Rules derived from GOT (proof not required). Setting up of character table of C_{2v}, C_{3v} and C_{2h} groups. Direct product representations. Reduction formula, reduction of reducible representation to IRs. Transformation properties of atomic orbitals. Hybridisation: identification of atomic orbitals taking part in hybridisation of triangular planar, square planar, trigonal bipyramidal, square pyramidal and tetrahedral molecules. Molecular symmetry and optical activity.

Unit IV Isopoly and heteropoly acids, Noble gases, interhalogens   18 h

Preparation, properties and structure of isopoly acids of Mo,W and V and Heteropoly   acids of Mo and W. Preparation and properties of Xenon fluorides and Krypton compounds ($KrCl_4$, KrF_4, KrF_2, $KrBr_6$, $Kr_2Cr_2O_7$, $KrCrO_4$ & KrO_2), structure of XeF_2 (MO theory only) . Preparation, bonding and uses of inter halogen compounds. Properties and structure of aluminosilicates and zeolites, shape selectivity. Preparation, properties and applications of silicones.

Unit V Chemistry of Natural Environmental Processes   18 h

The chemistry of processes in atmosphere; Composition of the atmosphere. Automobile pollutants and the catalytic converter. Photochemical smog. Chemistry of the stratosphere. Catalytic destruction of ozone. Depletion of the ozone layer. Hazards of common air pollutants on the human health. The Chemistry of processes in hydrosphere; The hydrologic cycle. Cycling and purification. The unique properties of water. Acid base properties. CO_2 in water. Alkalinity. O_2 consuming waste. DO, BOD and COD. The chemistry of processes in Lithosphere; Redox status in soil. pE, pH predominance diagrams for redox sensitive elements. Acidity in soil materials. Acid neutralization capacity and the quantification of the soil acidity. Ion speciation in soil solution. Cation exchange capacity and exchange phase composition.

References

1.   F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, John Wiley and Sons, 6th edition, 1999.

2.   J. E. Huheey, Inorganic Chemistry- Principles of Structure and Reactivity, Harper Collins College Publishing, 4th edition, 2011.

3. K. F. Purcell and J. C. Kotz, Inorganic Chemistry, Saunders, 1977.

4. S. F. A. Kettle, Physical Inorganic Chemistry, Oxford University Press, 1st edition, 1998.

5. Shriver and Atkins, Inorganic Chemistry, Oxford University Press, 2010.

6. A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 5th edition, 1989.

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9. F.A.Cotton, Chemical Applications of Group Theory, Wiley Eastern, 3rd edition, 2009.

10. A.S.Kunju and G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2010.

11. R.L.Carter, Molecular Symmetry and Group Theory, John Wiley& Sons,1998

12. E.James Girard, Principles of Environmental Chemistry, Jones and Bartlett Publishers, 3rd Edition, 2013

13. H.V. Jadhav, Elements of Environmental Chemistry, Himalya Publication House, 2010

14. E. Michael Essington, Soil and water Chemistry, CRC Press, 2nd edition, 2015

CM 212 ORGANIC CHEMISTRY-I

Total 90 h

Unit I Stereochemistry of organic compounds   **18h**

Nomenclature of organic compounds - Cyclic, fused polycyclic and bridged polycyclic hydrocarbons, Bridged and fused hydrocarbon systems, Spirocyclic hydrocarbon systems, Heterocyclic systems containing Nitrogen and Oxygen.

Introduction to molecular symmetry and chirality, Axial Chirality, Planar Chirality and Helicity, Relative configuration, Stereochemical nomenclature, *R* and *S*, *E* and *Z*. Prostereoisomerism, stereotopicity and stereoprojections. Non-carbon chiral centres –Nitrogen, phosphorus and sulfur as chiral centres.Axial stereochemistry:Atropisomerismand its designation, *M* and *P* configurations. Stereoselectivity: enatioseelctetivity, diastereeoselectivity and stereoconvergence. Basic introduction to chiral separation methods and estimation of enantiomeric excess.

Conformational analysis of alkanes and cycloalkanes, Biased systems. Effect of conformation on reactivity of cyclohexanes– conformation of decalin.

Introduction to ORD, CD- their application in assigning configuration.Sector rules such as octant and axial haloketone rules. Cotton effect.

Chiral drugs: Ibuprofen, Methyldopa, and Thalidomide – Structure, chirality and activity(Basic concepts only)

Unit II Structure, reactivity and intermediates   **18 h**

Reaction coordinates- difference between transition state and intermediates, Homolytic and heterolyticbond fissions. Formation and structure of carbocations, carbanion and free radicals, Stability of intermediates, influence of field effect, inductive, mesomericand steric effects on controlling stability if carbocations, carbanions and carbon-centered radicals. Influence of structural features on acidity, basicity and reactivity of organic compounds. Alkyl, aralkyl and allylic cations –influence of substituents. General reactions of carbocations, carbanions and free radicals.Introduction to radical ions. Formation, structure, stability and chemical reactions of carbens, nitrenes and arynes

Unit III Substitution reactions   18 h

Nucleophilic substitution at sp^3carbon - S_N1 and S_N2 mechanisms.Walden inversion, stereochemistry.Effect of solvent,leaving group and substrate structure on rates of S_N1 and S_N2 substitutions.Neighbouring group participation, Non-classical carbocations, Competition between S_N1 and $S_N2$reactions.S_N1', S_N2', S_Ni mechanism.

Mechanism of esterification and ester hydrolysis-acid catalysed and base catalysed reactions.

Aromatic Substitution reactions - Electrophilic substitution: mechanism and evidence- Reactions involving nitrogen, sulphur, carbon, halogen and oxygen electrophiles. Directive and rate controlling factors in aromatics with one or more substituents.

Aromatic Nucleophilic Substitution reactions - S_N1, S_NAr, benzyne and $S_{RN}1$ mechanism and evidence with examples.

Unit IV Elimination and addition reactions   18h

Elimination reactions leading to C=C bond formation and their mechanisms. E1, E2 and E1CB mechanisms.Stereoaspects of C=C bond formation. Effect of leaving group and substrate structure.Hoffmann and Saytzeff elimination.Cis elimination.Stereoaspects of the addition of H_2O, X_2, HX, and boranes to C=C systems.Effect of substituents on the rate of additions. Cis and trans hydroxylation of cycloalkenes. Nucleophilic addition to activated C=C systems. Structure of the transition state in the addition reactions. Michael addition:mechanism with evidence. Addition to Carbon-Heteroatom multiple bonds: Aldol condensation (normal, crossed and directed), Perkin, Stobbe, Knoevenagel, Darzen, Reformatsky and benzoin condensations. Grignard, Cannizzaro, Wittig and Wittig-Horner reactions.Application of Cram's rule, Felkin-Ann model.

Unit V Reagents in organic synthesis   18h

Applications of hydrogenation catalysts, hindered boranes, bulky metal hydrides. $NaCNBH_3$ DIBAL, Li trialkylborohydrides, tri-*n*-butyltin hydride, diimide, Lindlar catalysts and aluminium alkoxide. Rosenmund reduction and McFadeyan-Stevens reaction. Oxidation using SeO_2, lead tetraacetate, ozone, peracids, DDQ, manganese (1V) oxide, silver carbonate and Cr(V1) reagents. Swern oxidation, Moffatt oxidation, allylic and benzylic oxidation.Sommelet reaction.Elbs reaction.Oxidative coupling of phenols.Chemo and regioselectivity in reductions and oxidations.

References

1. D. Hellwinkel, Systematic nomenclature of organic chemistry, Springer, 2001.

2. D. Nasipuri, "Stereochemistry of Organic compounds", 2nd Edition, Wiley Eastern, 1994.

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17. W. Carruthers, "Modern methods in organic synthesis," 3rd Edition, Cambridge University Press, 1987.

18. R. O. C. Norman and J. M. Coxon, "Principles of organic synthesis," CRC Press, 1993.

CM213 PHYSICAL CHEMISTRY –I   90 hrs

Unit 1- Quantum Chemistry I   18 hrs

Failure of classical mechanics, need of quantum mechanics, concept of matter wave,de Broglie relation and its experimental proof, uncertainty principle and its consequences.

Postulates of Quantum Mechanics

State function postulate:Born interpretation of the wavefunction, well behaved functions, orthonormality of wave functions. Operator postulate: operator algebra, linear and nonlinear operators, Laplacian operator, commuting and non-commuting operators, Hermitian operators and their properties, eigen functions and eigen values of an operator. Eigen value postulate: eigen value equation, eigen functions of commuting operators. Expectation value postulate. Postulate of time-dependent Schrödinger equation, Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta (L_x, L_y, L_z and L^2)-commutation relations between these operators.

Application of Quantum mechanics to Exactly Solvable Model Problems

Translational motion: free particle in one-dimension, particle in a box with infinite potential barrier- one dimensional box, three dimensional box and cubical box - degeneracy -particle with finite potential barriers- one potential barrier,two finite barriers, potential barriers of definite thickness-Quantum mechanical tunneling (Qualitative concept only)

Vibrational motion: one-dimensional harmonic oscillator (complete treatment), Hermite equation (solving by method of power series), Hermite polynomials, recursion relation, wave functions and energies-important features, Harmonic oscillator model and molecular vibrations.

Symmetric and antisymmetric wave functions, Pauli's antisymmetry principle, the postulate of spin. Spin orbitals. Spin-orbit coupling.

Vector atom model- Term symbols, explanation of spectral lines (for s and p blocks only)

Unit II Surface Chemistry and Catalysis   18 hrs

The Gas- solid inter phase,types of adsorption. Heat of adsorption and its determination, differences betweenchemisorption and physisorption. Adsorption isotherms -classical,Freundlich and Langmuir isotherms. Thermodynamic and statistical derivation of Langmuir adsorption isotherm. Multilayer adsorption- the BET theory and Harkins- Juratheory.

Adsorption from solutions: Gibb's adsorption equation and its verification. Adsorption with dissociation. Adsorption with interaction between adsorbate molecules.

Different types of surfaces,Properties of surface phase. Thermodynamics of surface. Surface tension of solutions. Surfactants andmiscelles.Examination of surfaces using low energy electron diffraction, photoelectron spectroscopy, ESCA, scanning probe microscopy, Auger electron spectroscopy , SEM andTEM.

Surface films-different types, surface pressure and its measurement,surface potential and its measurementsand interpretation.Measurement of surface area of solids - Harkins – Jura absolute method, entropy method andthe point B method. Use of Langmuir, BET and Harkins – Jura isotherms for surface areadetermination.

Catalysis: Mechanism and theories of homogeneous and heterogeneous catalysis. Enzymecatalysis, bimolecular surface reactions. Langmuir – Hinshelwood mechanism, instrumental methods of catalyst characterization-diffraction and thermal methods,spectroscopic and microscopic techniques.

Unit 1II: Classical Thermodynamics 18 Hrs

Entropy- dependence of entropy on variables of a system (S, T and V; S,T and P). Thermodynamic equations of state. Criteria for equilibrium and spontaneity, Euler's relation, Gibbs and Helmholtz free energy, Maxwell relations and significance, temperature dependence of free energy, Gibbs Helmholtz equation and its applications.

Partial molar quantities:, chemical potential, Gibbs-Duhem equations, determination of partial molar properties –partial molar volume and partial molar enthalpy.

Fugacity- relation between fugacity and pressure, determination of fugacity of a real gas, variation of fugacity with temperature and pressure. Fugacity of liquid mixtures, fugacity of mixture of gases, Lewis Randall rule.

Activity, activity coefficients, dependence of activity on temperature and pressure. Determination of activity and activity coefficients of electrolytes and non electrolytes

Thermodynamics of mixing, Duhem-Margules equation, Konowaloff'srule, Henry's law, excess thermodynamic functions- Determination of excess enthalpy and volume.

Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium- van't Hoff reaction isochore and isotherm.

Unit IVChemical kinetics 18 hrs

Theories of reaction rates: Collision theory and its failure,. Transition state theory-Eyring equation. Comparison of the two theories. Thermodynamicformulation of the reaction rates. potential energysurfaces

Theories of unimolecular reactions- Lindemann theory,Lindemann-Hinshelwood mechanism, qualitative idea of RRKM theory,

Kinetics of complex reactions-parallel reactions,opposing reactions,consecutive reactions and chain reactions, steady state treatment, kinetics of H_2-Cl_2 and H_2-Br_2 reactions, decompositions of ethane , acetaldehyde and N_2O_5. Rice-Herzfeld mechanism, branching chain reactions Hinshelwood mechanism of chain reactions and explosion.

Fast reactions: Relaxation method, relaxation spectrometry, flow method, shockmethod, fast mixing method, field jump method, pulse method, Flash photolysis and NMRmethod.

Reactions in solution: Factors affecting reaction rates in solutions, effect ofdielectric constant and ionic strength, cage effect, Bronsted-Bjerrum equation,primary and secondary kinetic salt effect, influence of solvent on reaction rates,significance of volume of activation, linear free energy relationship. Hammet equation and Taft equation.

Photochemistry: Effect of radiation on the rate of reaction,Jebalonski diagram, Laws of photochemistry. Quantumyield. Experimental determination of quantum yield.Fluorescence and phosphorescence, Quenching of fluorescence, Stern-Volmer equation.

Unit V Gaseous and liquid state　　　　　18 hrs

Maxwell's distribution of molecular velocities, influence of temperature on molecular velocities, types of molecular velocities—average velocity and most probable velocity and its determination from Maxwell's equation

Transport phenomena in gases—viscosity of gases, Chapman equation, determination of viscosity of gases, calculation of mean free path, Thermal conductivity, diffusion, Degrees of freedom of gaseous molecules - Transilational, Rotational and vibrational. Equation of state of real gases—van der Waal's equation, Other equation of states—Radlich-Kwong equation, Clausius equation, Virial equation, second virial coefficient and determination of diameter of a molecule.

Inter molecular forces—dipole-dipole interaction, induced dipole- dipole, induced dipole-induced dipole interactions

Liquid state Liquid vapour equillibria, vapour pressure- methods of measuring vapour pressure - barometric method and dynamic method - equation of state for liquids, structure of liquids, X-ray diffraction of liquids-vacancy model for a liquid, pair correlation function, surface tension , determination of surface tension, drop weight method and drop number method, viscosity, determination of coefficient of viscosity using Ostwald viscometer.

References

1.　　I.N. Levin, "Quantum Chemistry", Prentice Hall

2.　　D. A. McQuarrie, "Quantum Chemistry", Viva Publishers.

3.　　M. W. Hanna, "Quantum Mechanics in Chemistry", Benjamin.

4.　　R. K. Prasad, "Quantum Chemistry", New Age International Publishers

5.　　T. Angel, "Quantum Chemistry and Spectroscopy",Pearson Education.

6.　　P. W. Atkins , R. S. Friedman, "Molecular Quantum Mechanics", Oxford University Press.

7.　　J. P Lowe, K. Peterson, "Quantum Chemistry", New Age International

8.　　S. Glasstone, "Thermodynamics for Chemists",

9.　　G.W.Castellan, "Physical Chemistry", Addison-Lesley Publishing.

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16.　　K.K Rohatgi-Mukherjee, "Fundamentals of Photochemistry", New age International.

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18.　　D.K. Chakrabarty and B. Viswanathan, Heterogeneous catalysis, New Age Publications .

19.　　G. A.Somorjai.Y.Li, Introduction to Surface Chemistry and Catalysis.International

20.　　Puri, Sharma, Pathania," "Principles of physical Chemistry" Vishal publishing company.

21.　　Gurdeep Raj "Advanced Physical Chemistry" GOEL Publishing House, Meerut.

C

CM 214 –INORGANIC CHEMISTRY PRACTICALS -1

Total 125 h

1. Separation and identification of rare/less familiar cations such as Ti, W, Mo, Th, Zr, V, U and Li

2. Volumetric estimation using EDTA, ammonium vanadate, ceric sulphate etc.

3. Colorimetric estimation of Cr, Fe, Mn, Ni, Cu etc.

4. Preparation of metal complexes: selection can be made from the following or any other from the existing literature.

· $[Co(NH_3)_6]Cl_3$

· $[Cu(NH_3)_4]SO_4$

· $K_3[Cr(C_2O_4)_3]$

· $K_3[Fe(C_2O_4)_3]$

· Cis and trans isomers of $[Co(en)_2Cl_2]Cl$

· $[Cr(en)_3]Cl_3$

References

1. A. I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 4th edition, 1978.

2. A. I. Vogel, A Text Book of Qualitative Inorganic Analysis, Longman 5th edition, 1979.

3. D.A. Skoog and D. M. West, Analytical Chemistry: An Introduction, Saunders College Publishing, 4th edition, 1986.

4. W. G. Palmer, Experimental Inorganic Chemistry, Cambridge University, 1959.

CM 215 ORGANIC PRACTICALS-1

Total 125 hrs

A . Separation and identification of organic compounds

1. Quantitative wet chemistry separation of a mixture of two components by solvent extraction

2. TLC of the purified samples along with the mixture in same TLC **plates (component 1 with mixture and component 2 with mixture on separate TLC plate) and** calculation of R_f values- Reporting and recording TLC in standard formats- preparation of sample solution, adsorbent, dimensions of the plate, saturation time, developing time, visualization and detection, R_f Value, Drawing - in the form of a table.

B. Separation of a mixture of by column chromatography (not for End semester evaluation)

1) Malachite green and methylene blue 2) *o*-nitroaniline and *p*-nitroaniline.

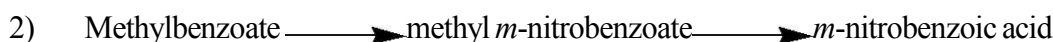### C. Preparation of compounds by two stages.

Recording/downloading UV,IR,^{1}H NMR and ^{13}C NMR and EI mass spectra of synthesized compounds.

TLC analysis- stage 1 reactants and products on TLC plate 1 and stage 2 reactants and products on plate 2)- Record TLC in standard format as in separation

All preparations must be restricted to 1 g level

Nitration

1)   Acetanilide-———➤*p*-nitroacetanilide———➤*p*-nitroaniline

2)   Methylbenzoate ⟶ methyl *m*-nitrobenzoate ⟶ *m*-nitrobenzoic acid

Bromination

3) Acetanilide- ⟶ *p*-bromoacetanilide ⟶ *p*-bromooaniline

Aldol condensation- Synthesis of heterocycles

4)   benzaldehyde ⟶ Dibenzylideneacetone ⟶ 1,5-Diphenyl-3-styryl-2-pyrazoline

Diazocoupling

5)   Aniline ⟶ Diazoaminobenzene ⟶ *p*-aminoazobenzene

Rerrangement

6)   Pthalic anhydride - ⟶ Pthalimide ⟶ anthranilic acid

Synthesis of Dyes

7)   N,N-Dimethylaniline ⟶ N,N-dimethyl-4-nitrosoaniline - ⟶ methylene blue

The board of examiners have to select either TLC of separated components *OR* TLC of preparation for an examination. But both TLC examinations are to be practiced and entered in the record of experiments.

References

1.   B. S. Furniss, "Vogel's text book of practical organic chemistry," 5th Edition, Longman, 1989.

2.   D. L. Pavia, G. M. Lampman, G. S. Kriz and R. G. Engel, "A microscale approach to organic laboratory techniques," Wadsworth Publishing, 5th Edition, 2012.

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4.   N. K. Vishnoi, "Advanced Practical Organic Chemistry," 3rd Edition, Vikas

5.   F. G. Mann and B. C. Saunders, "Practical Organic Chemistry," Pearson Education, 2009

6.   J. B. Cohen, "Practical organic chemistry," Forgotten Books, 2015

7.   P. F Shalz, *Journal of Chemical Education* 1996, *173*: 267.

8.   Monograph on green laboratory experiments, DST, Government of India, pp 1-79.

9.   For spectral data of organic compounds, see: **http://sdbs.riodb.aist.go.jp/sdbs/cgi-bin/direct frame top.cgi.**

CM 216 PHYSICAL PRACTICALS –I

125 hrs

Adsorption

Freundlich and Langmuir isotherms for adsorption of acetic/oxalic acid on active charcoal.

Determination of concentration of acetic/ oxalic acid.

Kinetics

Determination of rate constant of acid hydrolysis of methyl acetate.

Determination of Arrhenius parameters.

Determination of concentration of given acid.

Determination of rate constant of the saponification of ethyl acetate and evaluation of Arrhenius parameters.

Determination of rate constant of reaction between $K_2S_2O_8$ and KI.

Study the kinetics of iodination of acetone in acid medium.

Phase rule

Solid-liquid equilibria

Construction of phase diagram and determination of the composition of unknown mixture (naphthalene/biphenyl, naphthalene/benzophenone, naphthalene/diphenyl amine)

Construction of phase diagram with congruent melting point- naphthalene/metadinitrobenzene

Partially miscible liquid pairs- CST of phenol-water system.

Effect of impurities (KCl/ NaCl/ succinic acid) on the miscibility temperature of phenol-water system and hence the determination of concentration of given unknown solution.

Three component system- Construction of ternary phase diagram of acetic acid chloroform-water system and hence the composition of given homogeneous mixture. Construction of tie-line.

Distribution law

Distribution coefficient of ammonia between chloroform and water.

Determination of equilibrium constant of copper- ammonia complex by partition method or coordination number of Cu^{2+} in copper-ammonia complex.

Distribution coefficient of benzoic acid between toluene and water.

Distribution coefficient of iodine between hexane and water/$CHCl_3$ and water/ CCl_4 and water

Determination of the equilibrium constant of the reaction $KI + I_2$ ”![KI_3] and hence the

concentration of given KI in hexane and water/$CHCl_3$ and water/ CCl_4 and water.

Determination of hydrolysis constant of anilinium hydrochloride.

Dilute Solutions

Determination of K_f of solid solvent, molar mass of non-volatile solute, mass of solvent

and composition of given solution (Solvent- Naphthalene/Biphenyl/ Benzophenone etc.

Solute- Naphthalene/ Biphenyl/ Diphenylanmine etc)

Determination of vant Hoff's factor for benzoic acid in Naphthalene.

Determination of atomicity of sulphur.

Transition temperature

Determination of K_T of salt hydrate, molar mass of solute, mass of salt hydrate and

composition of given solution (Solvent- $Na_2S_2O_3.5H_2O$/$CH_3COONa.3H_2O$, Solutes glucose,sucrose, urea)

Thermochemistry

Determination of the concentration of given strong acid/alkali.

Thermometric titration of NaOH Vs standard HCl.

Heat of displacement of Cu^{2+} by Zn.

Determination of the heat of ionisation of acetic acid.

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First Semester M.Sc. Degree Examination – Model question paper

Branch – Medicinal Chemistry

CM 211 : INORGANIC CHEMISTRY- I

(2016 Admission Onwards)

(Common for CH/CL/CA/CM 211)

Time : 3 Hrs   Max. Marks: 75

SECTION A

Answer **two** among **(a), (b)** and **(c)** from **each** question carries **2** marks

1. a) What is meant by Nephelauxetic effect?

    b) Explain linkage isomerism with suitable example.

    c) What is meant by crystal field stabilization energy?

2. a) What do you mean by significant figure? How many significant figures are in the following?

    i)   0.0026

    ii) 6.023×10^{23}

    b) What are metallochromic indicators? Give an example.

    c) In a volumetric experiment the volumes of the titrant used are 9.98, 9.99, 9.98, 9.95, 10.00 and 10.02 mL. Calculate the standard deviation.

3. a) Identify the symmetry elements present in the following and assign the point group   i) H_2O ii) HCl

    b) Explain improper axis of symmetry.

    c) What is meant by character table.

4. a) Explain the term 'shape selectivity'.

    b) Give the preparation of $KrCl_4$ and KrO_2.

    c) What are zeolite? Explain their use as water softeners.

5. a) Brief the role of catalytic converters in automobiles.

    b) Explain the formation of photochemical smog.

    c) Mention the different regions of atmosphere.   **(2x10= 20 marks)**

SECTION B

Answer either among **(a) or (b)** from **each** question carries **5** marks

6. a) State and illustrate Jahn Teller effect.

b) Explain the crystal field theory of octahedral complexes.

7. a) Give a brief note on scatter diagram and its significance.

b) Explain the titrations in non-aqueous solvents.

8. a) Construct the multiplication table for the symmetry operations of NH_3 molecule.

b) State and explain orthogonality theorem.

9. a) Give an account of inter halogen compounds.

b) Write a short note on silicones.

10. a) List out the major pollutants. Outline how they affect human health?

b) Describe how we can quantify soil acidity.   **(5x5= 25 marks)**

SECTION C

Answer **any three** questions. **Each** question carries **10** marks

11. Explain the bonding in octahedral complexes with and without pi bonds using MO Theory.

12. Briefly explain the principle, instrumentation and applications of TG and DTA.

13. Construct the character table for C_{2v} and explain.

14. Write a short note on the preparation and properties of heteropoly acids of Mo and W.

15. What are Pourbaiux diagrams? Outline its role in explaining the chemistry of processes in lithosphere.

(10x3= 30 marks)

FIRST SEMESTER MSc.DEGREE EXAMINATION
BRANCH – MEDICINAL CHEMISTRY
CH/CL/CA/CM212: Organic Chemistry-I
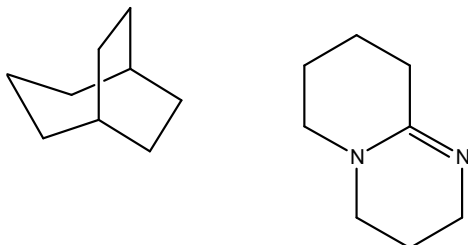## (2016 admission)

Time: 3 hours   Maximum marks:75

Section A

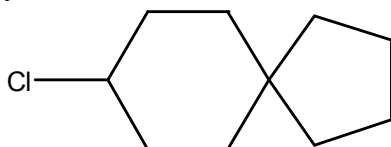**Answer any two among (a), (b) and (c) from each question. Each sub question carries 2 marks**

1   a) Write IUPAC names of the following.
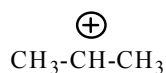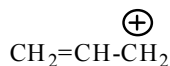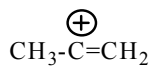
b) Indicate the element of symmetry present in each of the following molecules.

i) *trans*-1,4-dichlorocyclohexane-

ii) -

c) What is atropisomerism?

2. a) How arynes are formed?

b) *p*-Nitroaniline is less basic than *m*-nitroanile, explain.

c) Arrange the following carbocations in order of increasing stability and give reasons.

$$CH_3-\overset{\oplus}{C}=CH_2 \qquad CH_2=CH-\overset{\oplus}{C}H_2 \qquad CH_3-\overset{\oplus}{C}H-CH_3$$

3. a) What is SNi reaction?

b) Alkaline hydrolysis of $Et_2NCH(Cl)CH_2CH_3$ produces $Et_2NCH(Et)CH_2OH$. Account for this observation

c) Write two examples of non classicalcarbocations.

4 a) How would you prepare trans-1,2-dihydroxycyclohexane from cyclohexene?

b) Write the mechanism of benzoin condensation.

c) How can the E1CB pathway be distinguished from the kinetically indistinguishable E2 pathway?

5 a) Write two important reaction of $NaCNBH_3$

b) Explain the importance of DDQ in organic synthesis.

c) Explain Swern Oxidation   **(2x10= 20 marks)**

Section B

Answer either (a) or (b) from each question. Each sub question carries 5 marks

6 a) Compare ORD and CD and explain their relationship

b) Write a note on stereochemistry of nitrogen compounds

7 a) Explain the Felkin-Ann model with an example

b) How carbenes are generated? Explain its structure and properties

8 a) Explain why anti Markonikoff's addition is not exhibited by HCl or HI when reacted with 1-butene?

b) After standing in aqueous acid *R*-2-butanol is found to have lost its optical activity. Account for this observation.

9 a) Write a note on cis and trans hydroxylation of alkenes

b) State Crams rule.Explain it with suitable example

10 a) Write a note on oxidation using SeO_2

b) Explain briefly the role of Lead tetra acetate in organic synthesis   **(5x5= 25 marks)**

Section C

Answer **any three** questions. **Each** question carries **10** marks

11. Give a brief account on stereoselectivity, enantiomeric excess and chiral separation.

12 Explain the following

a. S_NAr mechanism , b) Orientation effect in aromatic electrophilic substitution

13. Discuss the following

a) competition between S_N1 and S_N2 b) Stereochemistry of nucleophilic substitution

14. Describe the following

    a) Mechanism with evidences of aldol condensation

    b) Wittig reactions and applications

15. Write a note on a) Sharpless asymmetric epoxidation

    b) Chemoselectivity in reduction reactions   **(10x3= 30 marks)**

First Semester M.Sc. Degree Examination (Model Question Paper)
Branch-Medicinal Chemistry
CM 213/CH 213/CL 213/CA 213 : Physical Chemistry- 1
(2016 Admission Onwards)

I

Time: 3 h   Max.Marks:75

Section A

Answer any two from **a,b,c**, of each question. Each sub question carries **2** marks.

(10 x 2 = 20 marks)

1. (a) Calculate de Broglie wave length of mass 1 mg moving with a velocity of 10 m s^{-1}

   (b) What is an operator? Give example.

   (c) Write spectroscopic term symbol for the ground state of O atom

2. (a) What is the principle of photoelectron spectroscopy?

   (b) Write the B.E.T theory of multilayer adsorption kjhh

   (c) Write the different types of adsorption ?Explain

3. (a) Define chemical potential

   (b) State Lewis –Randall rule of fugacity

   (c) Write Konowaloff's rule

4. (a) How is nmr spectroscopy made use of in the study of fast reactions?

   (b) What is steady state approximation?

   (c) Define quantum yield

5. (a) What is the effect of temperature on the distribution of molecular velocities of a gas? Explain.

   (b) Calculate the root mean square velocity of nitrogen atn27^{0}C

   (c) Write the virial equation of state. Explain the terms

Section B

Answer either **a** or **b** of each question. Each question carries **5** marks.

(5 x 5 = 25 marks)

6. (a) Explain Quntaum mechanical Tunneling

   (b) Write kinetic energy operator. Show that it is a Hermition operator

7. (a) Write any two methods for the determination of surface area of a solid

   (b) Explain Langmuir-Hinshelwood mechanism of surface catalysed reaction

8. (a) Define fugacity. Write the method for the determination of fugacity of a gas

    (b) Derive Gibbs Duhem equation

9. (a) Explain Jabalonski diagram

    (b) Derive the rate law for the decomposition of N_2O_5

10. (a) Calculate the viscosity of O_2 at 25^0C. The molecular diameter is 3.6A

    (b) Write any one method for the determination of surface tension of liquid

Section C

Answer any **three** questions. Each question carries **10** marks.   (3 x 10 = 30 marks)

11. Apply Schrodinger Wave equation for a simple harmonic oscillator. Find eigen values and eigen functions

12. Explain any two methods using for surface analysis

13. Write a brief account of the methods for the determination of activity coefficient of electrolytes and non electrolytes

14. Explain chain reactions. Discuss Seminoff Henshelwood theory of branching chain reactions

15. Discuss viscosity of a gas and Chapman equation. How can we calculate mean free path and collision diameter from viscosity determination

SEMESTER II

CM 221 INORGANIC CHEMISTRY –II

Total 90 h

Unit I Sulphur, nitrogen, phosphorus and boron compounds   18 h

Sulphur-nitrogen compounds: Tetrasulphur tetranitride, disulphur dinitride and polythiazyl S_xN_y compounds. S-N cations and anions. Sulphur-phosphorus compounds: Molecular sulphides such as P_4S_3, P_4S_7, P_4S_9 and P_4S_{10}. Phosphorous-nitrogen compounds: Phosphazines. Cyclo and linear phosphazines. Boron-nitrogen compounds: Borazine, substituted borazines and boron nitride. Boron hydrides: Reactions of diborane. Structure and bonding. Polyhedral boranes: Preparation, properties, structure and bonding. The topological approach to boron hydride structure. *Styx* numbers. Importance of icosahedral framework of boron atoms in boron chemistry. Closo, nido and arachno structures.Wade's rules. Carboranes and metallocarboranes.

Unit II Coordination chemistry-II: Spectral and magnetic properties of transition metal complexes 18 h

Electronic spectra of metal complexes- Term symbols of d^n system, Racah parameters, splitting of terms in weak and strong octahedral and tetrahedral fields. Correlation diagrams for d^n and d^{10-n} ions in octahedral and tetrahedral fields (qualitative approach), *d-d* transition, selection rules for electronic transition-effect of spin orbit coupling and vibronic coupling Interpretation of electronic spectra of complexes- Orgel diagrams, Tanabe-Sugano diagrams, Calculation of *Dq , B* and â (Nephelauxetic ratio) values, charge transfer spectra. Magnetic properties of complexes-paramagnetic and diamagnetic complexes, molar susceptibility, Gouy's method for the determination of magnetic moment of complexes, spin only magnetic moment. Temperature dependence of magnetism. Temperature Independent Paramagnetism (TIP). Spin state crossover, Antiferromagnetism-inter and intra molecular interaction. Application of magnetic measurements in the determination of structure of transition metal complexes.

Unit III Crystalline state   18 h

Crystal systems and lattice types. Bravais lattices. Crystal symmetry- Introduction to point groups and space groups. Miller indices. Reciprocal lattice concept. Close packed structures: BCC, FCC and HCP . Voids. Coordination number. Crystal binding: Molecular, covalent, metallic and hydrogen bonded crystals.

X- Ray diffraction by crystals: Function of crystals. Transmission grating and reflection grating. Braggs equation. Diffraction methods: Powder and rotating crystal. Indexing and determination of lattice type and unit cell dimensions of cubic crystals. Crystal defects: Perfect and imperfect crystals. Point, line and plane defects. Thermodynamics of Schottky and Frenkel defects. Colour centers in alkali halide crystals. Defect clusters. Extended defects: Crystallographic shear structure and stacking faults. Dislocations and crystal structure. Structure of compounds of AX (Zinc blende, Wurtzite) , AX_2 (Rutile, fluorite, antifluorite), A_mX_2 (Nickel arsenide), ABX_3 (Perosvskite, Ilmenite). Spinels. Inverse spinel structures.

Unit IV Lanthanides and actinides   18 h

Lanthanides: Characteristic properties. Electronic configurations and term symbols. Occurrence and extraction. Separation techniques. Oxidation states. Spectral and magnetic properties. Shapes of f orbital and their splitting in cubic ligand field. Lanthanide complexes as shift reagents. Actinides: Occurrence and general properties. Extraction of thorium and uranium. Electronic configuration and term symbol. Oxidation states. Spectral and magnetic properties. Comparative properties of lanthanides and actinides. Trans-uranium elements and their stabilities. Applications of lanthanide and actinide compounds. Comprehensive study of the beach sands of Kerala and their important components such as monazite, ilmenite, zircon and sillimanite.

Unit V Solid state chemistry   18 h

Electronic structure of solids. Free electron theory, band theory. Refinements to simple band theory, k space and Brillouin zones. Conductors, insulators and semiconductors. Band structure of conductors, insulators and semiconductors and their applications. Intrinsic and extrinsic semiconductors, doping of semiconductors and conduction mechanism, the band gap, temperature dependence of conductivity, carrier density and carrier mobility in semiconductors, Superconductivity, Photoconductivity, Photovoltaic effect. Colour in inorganic solids. Dielectric properties. Dielectric materials. Ferroelectricity, pyroelectricity, piezoelectricity and ionic conductivity. Applications of ferro, piezo and pyroelectrics.

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1.   F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, John Wiley and Sons, 6th edition, 1999.

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3.   S. F. A. Kettle, Physical Inorganic Chemistry, Oxford University Press, 1st edition, 1998.

4.   A. R. West, Solid State Chemistry and its Applications, Wiley Eastern, 1990.

5.   H. J. Emeleus and A. G. Sharp, Modern Aspects of Inorganic Chemistry, Van Nostrand, 4th edition,1973.

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10.   C. Kittel, Introduction to Solid State Physics, Wiley and Sons, 8th edition, 2004.

11.   N. N. Greenwood and A. Earnshaw, Chemistry of Elements, REPP Ltd, 2nd edition, 2005.

12.   A. Earnshaw, Introduction to Magnetochemistry, Academic Press, 1968.

CM 222 ORGANIC CHEMISTRY- II

Total 90 h

Unit I Physical organic chemistry18 h

Reactivity in relation to molecular structure and conformation.Steric effects.*F* strain.Ortho effect, Bond angle strain.Linear free energy relationships.The Hammett equation and its applications.Taft equation.Solvent polarity and parameters.Y, Z and E parameters and their applications.Primary and secondary kinetic isotope effects.Salt effects and special salt effects in SN reactions.Kinetic and thermodynamic control of reactions. Energy profiles, Hammond postulate. Principle of microscopic reversibility.Marcus theory.Methods of determining reaction mechanisms. Phase transfer catalysis and its applications.

Unit II Molecular rearrangement and transformation reactions18h

Types of organic rearrangements: Anionic, cationotropic, prototropic, free radical, carbene and nitrene intermediates. Mechanism with evidence of Wagner-Meerwein, Pinacol, Demjanov, Hofmann, Curtius, Schmidt, Lossen, Beckmann, Wolf, Fries, Fischer-Hepp, Hofmann-Martius, von-Richter, Orton, Bamberger, Smiles, Dienone-phenol, Benzilic acid, Benzidine, Favorskii, Stevens, Wittig, Sommelet-Hauser, Bayer-Villiger rearrangements.

Unit III Aromaticity and symmetry controlled reactions18 h

Aromaticity and antiaromaticity.Homo, hetero and non-benzenoid aromatic systems. Aromaticity of annulenes, mesoionic compounds, metallocenes, cyclic carbocations, carbanions.

Symmetry properties of MOs. Classification of pericyclic reactions.Mechanism and stereochemistry of electrocyclic, cycloaddition and sigmatropic reactions. Woodward- Hoffmann rules. FO, CD and Huckel-Mobius analysis of electrocyclic, cycloaddition and sigmatropic reactions.FO analysis of [1, j] and [3, 3] migrations. 1,3-dipolar cycloaddition. Stereo aspects of Diels-Alder reaction and Cope re arrangement.Intramolecular Diels-Alder, Retro Diels-Alder, Alder-ene, retro-ene andcheletropicreactions.Synthetic applications of Diels-Alder reactions.Fluxional molecules.

Unit IV Organic photochemistry18 h

Photochemical processes.Energy transfer, sensitization and quenching.Singlet and triplet states and their reactivity.Photoreactions of carbonyl compounds, enes, dienes and arenes.Norrish Type I and Type II reactions of acyclic ketones. Free radical reactions:Patterno-Buchi and Barton reactions, photo-Fries and Di-π methane rearrangements. Photoreactions of Vitamin D. Photosynthesis, photochemistry of vision.Singlet oxygen generation and their reactions.Introduction to chemiluminescence.Applications of photochemistry.

Unit V Chemistry of natural products and biomolecules18 h

Introduction to primary and secondary metabolites in plants.Extraction methods of chemical constituents from plants, such as fractionation using solvents, specific extraction of alkaloids and supercritical fluid extraction.Characterizations of isolated compounds (terpenes, sterols, alkaloids, carbohydrates, flavonoids and poly phenols) by colour reactions and spray reagents.Biosynthesis of terpenes from mevalonic acid and sterols from squalene. Structure elucidation of ocimene, classification of pigments, structure elucidation of β-carotene. Structural differences between a triterpene and a sterol.Synthesis of quercetin, synthesis of testosterone, androsterone, estrone and progesterone.Determination of carbon skeleton of alkaloids (Hofmann, Emde and Von Braun degradation methods).Structural elucidation of ephedrine, nicotine, atropine.

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1.   L. M. Harwood, "Polar rearrangements," Oxford University Press 1995.

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J. Clayden, N. Greeves, and S. Warren, "Organic Chemistry," 2nd Edition, Oxford University Press, 2012.

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CM 223 PHYSICAL CHEMISTRY –II   90 Hrs

Unit I

Quantum Chemistry II

18 hrs

Rotational motion: Cartesian and spherical polar coordinates. The wave equation in spherical polar. coordinates - particle on a ring, the phi equation and its solution, wave functions in. the real form. Non-planar rigid rotor (or particle on a sphere)-separation of. variables, the phi and the theta equations and their solutions, Legendre and. associated Legendre equations, Legendre and associated Legendre polynomials. . Spherical harmonics (imaginary and real forms)-polar diagrams of spherical. harmonics

Quantum Mechanics of Hydrogen-like systems-Potential energy of hydrogen-like systems. The wave equation in spherical polar. coordinates: separation of variables-R, theta and phi equations and their solutions, . wave functions and energies of hydrogen-like systems. . Orbitals-radial functions, . radial distribution functions, angular functions and their plots**.** . Wave equation for multielectron. systems**.** Hartree-Fock Self-Consistent Field (HF-SCF) method for atoms, Hartree-Fock equations (derivation not required) & the Fock operator

Unit II Spectroscopy –I   18 hrs

Microwave spectroscopy: Rotational spectrum, intensity of spectral lines, calculation of internuclear distance. Non-rigid rotors and centrifugal distortion. Rotational spectra of polyatomicmolecules-linear and symmetric top molecules. Introduction to instrumentation.

Vibrational Spectroscopy: Vibrational spectra of harmonic and anharmonic oscillator.Selection rules. Morse curve, fundamentals and overtones. Determination of force constant.Rotational fine structure, P,Q,R branches

of spectra.Vibrational spectra of polyatomic molecules: Normal modes, classification of vibrationalmodes into stretching (asymmetric, symmetric), bending, parallel and perpendicularvibrations. Finger print region and group frequencies. Introduction to FTIR andinstrumentation.

Raman spectroscopy: Raman scattering, polarisability and classical theory of Ramanspectrum. Rotational and vibrational Raman spectrum. Raman spectra of polyatomicmolecules. Complementarity of IR and Raman spectra. Mutual exclusion principle.Introduction to instrumentation. Laser Raman spectrum.

Electronic spectra. Electronic spectra of diatomic molecules. Vibrational coarse structure androtational fine structure of electronic spectrum. Franck-Condon principle. Types of electronictransitions. Fotrat diagram. Predissociation . Calculation of heat of dissociation.Electronic spectra of polyatomic molecules: Electronic transition among molecular orbitalsand absorption frequencies. Effect of conjugation. Introduction to instrumentation.Simultaneous determination of two components.

Unit III Applications of Thermodynamics   18 hrs

Thermodynamics of irreversible processes: Simple examples of irreversible processes. General theory of non equilibrium processes The phenomenological relations. Onsager reciprocal relation. Generalized equation for entropy production, Entropy production from heat flow, matterflow and current flow.. Application of irreversible thermodynamics - to diffusion. Thermal diffusion, Thermo osmosis and thermomolecular pressure difference. Electro kinetic effects, the Glansdorf- Pregogine equation. Far from equilibrium region. Principle of minimum entropy production, Le-Chatelier Bra(u)wn Principle.

Three component systems : Graphical representation. Three component liquid systems with one pair of partially miscible liquids. Influence of temperature. Systems with two pairs and three pairs of partially miscible liquids.

Solid- Liquid systems: Two salts and water systems- no chemical combination, double salt formation, one salt forms a hydrate, double salt forms hydrate, Isothermal evaporation.

Unit IV Statistical Mechanics –I   18 hrs

Microstates. Concept of ensembles Canonical and Grand canonical ensemble. Classical distribution of particles-Maxwell Boltzmann distribution.

Bose-Einstein statistics, Bose-Einstein distribution. Thermodynamic probability, Bose Einstein distribution function. Examples of particles. Theory of Para magnetism. Bose Einstein condensation, Liquid Helium. Super cooled liquid.

Fermi- Dirac Statistics. Fermi- Dirac distribution, examples of particles Fermi-Dirac distribution functionThermionic emission. Relation between Maxwell Boltzmann, Bose Einstein and Fermi -Dirac Statistics.

Unit V Electrochemistry 1   18 hrs

Ionics- Ions in solution. Deviation from ideal behaviour. Ionic activity. Ion-solventinteraction. Born equation. Ion-ion interaction. Strong electrolytes Debye-Huckel theory of strong electrolytes,Onsager equation. Limitation of the model Conductance at highfrequencies and high potentials –Wein effect—Activity coefficient and its determination.

Ionic strength, Debye-Huckel limiting law. Equation for appreciable concentration. Osmotic coefficient. Activities in concentrated solutions. Ion associations.. Ion transport.

Electrodics: Different type of electrodes. Origin of electrode potential, Electrochemical cells, Concentration cells andactivity coefficient determination. Liquid junction potential. evaluation of thermodynamic properties, the electrode double layer, Electrode-electrodeinterface. Theory of multilayer capacity. Electrocapillarity. Lippmann potential andmembrane potential.

Electrokinetic phenomena. Mechanism of charge transfer at electrode- electrolyte interface.Electrolysis. Current- potential curve. Dissolution, deposition and decomposition potentials.Energy barriers at metal –

electrolyte interface. Different types of overpotentials. Butler-Volmer equation. Tafel and Nernst equation. Rate determining step in electrode kinetics. Thehydrogen and oxygen over voltage. Theories of overvoltage.

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SECOND SEMESTER MSc.DEGREE EXAMINATION

Branch:Medicinal Chemistry

(Common for CH/CL/CA/CM 221)

(Under Semester System w.e.f 2016 Admissions)

CM 221- INORGANIC CHEMISTRY-II

Time:3 h   Max marks:75

SECTION-A

Answer any two among (a), (b), and (c) from each question. Each sub-question carries 2 marks.

1. a) Classify the following as closo, nido, arachno or hypho.

   1) B_5H_9 2) B_5H_{11} 3) B_6H_{12} 4) B_9H_{15}.

   b) Which sulphur –nitrogen compound is known as 'one-dimensional' metal? Why is it called so?

c) Why are $P_4N_4C_{l8}$ puckered and $P_4N_4F_8$ planar?

2. a) How would you distinguish between ferro magnetic and anti ferromagnetic material?

b) Explain non-crossing rule.

c) The effective magnetic moment of a complex is 4.90 BM. Calculate the no: of unpaired electron per unit complex.

3. a) What is the type of defect observed in AgBr crystals? Why?

b) Give one example each for molecular, covalent, metallic and H-bonded crystals.

c) Differentiate between H-centre and v-centre in NaCl crystals.

4. a) Write any two differences between 4f and 5f orbitals.

b) Give the term symbols for Eu^{3+} and Lu^{3+}.

c) Explain why Actinides have greater tendency for complex formation than lanthanides?

5. a) What is band gap?

b) Draw the first Brillouin zone for a primitive cubic lattice?

c) Conductivity of metals decreases with increase of temperature. Explain.

[2 x 10 = 20 marks]

SECTION-B

Answer either (a) or (b) of each question carries 5 marks.

6. a) How is diborane prepared? Discuss the structure and bonding in diborane.

b) Write a note on metallocarboranes.

7. a) Describe the Guoy's method to determine magnetic susceptibility . How are these measurements used to calculate effective magnetic moments?

b) Even though d-d transitions are forbidden, why such transitions occur in many transition metal complexes? Illustrate with examples.

8. a) Distinguish between spinels and inverse spinels with suitable examples.

.b) Write briefly on line and plane defects in solids.

9. a) Briefly discuss the basis of the ion-exchange method for the separation of Lanthanides.

b) Compare the spectral and magnetic properties of Lanthanides and Actinides.

10. a) With suitable examples explain the phenomenon of photoconductivity. What are its applications?

b) Write a short note on the applications of ferro, piezo and pyroelectrics.

[5x 5 = 25 marks]

SECTION-C

Answer any three questions and each question carries 10 marks.

11. How is Borazine prepared? Discuss its structure and compare the bonding with phosphazene molecule.

12. Write an account on the selection rules and characteristics of d-d transition and application of each electronic spectra in elucidating the structure of metal complexes.

13. Discuss briefly on the packing of atoms and ions in solids.

14. a) Correlate the oxidation states and ionic radii with electronic configuration of lanthanides.

b)Write a short note on the beach sands of kerala.

15. Discuss the salient features of band theory of solids and compare it with the free electron theory of solids.

[10x3 = 30 marks]

SECOND SEMESTER MSc.DEGREE EXAMINATION
BRANCH – MEDICINAL CHEMISTRY
CH/CL/CA/CM222: Organic Chemistry-II
(Under Semester System w.e.f 2016 Admissions)

Time-3 hours   **Maximum marks: 75**

Section A

Answer any two among a), b) and c) from each question.

Each sub-question carries, 2 marks.

1. a) Give the mechanism of rearrangement of aryl hydroxylamines to aminophenols.

    b)Describe Stevens rearrangement.

    c)Show the mechanism involved in the rearrangement of an unsubstituted amide to a primary amine.

2. a) Explain why cyclodecapentaene with 10 ð electrons is not aromatic.

    b)Write briefly on Homoaromaticity.

    c) State Woodward Hoffmann rules.

3. a) Explain Phosphorescence.

    b) Write a short note on Norrish type I reaction.

    c) Describe anyone method of generation of singlet oxygen.

4. a) Explain von Braun reaction.

    b)Show the products formed when Quercetin is treated with dimethyl sulphate followed by boiling with ethanolic KOH.

    c)Draw the structure of CholesteroI.

5. a) Explain Taft equation

    b) Describe salt effect in substitution reaction

    c) State Marcus theory   **[2x10=20 marks]**

Section B

Answer either a) or b) of each question, and each question carries 5 marks.

6. a) Discuss the mechanism and applications of Baeyer Villiger reaction.

    b) Discuss the mechanism of Benzidine rearrangement. Also write proof to support the mechanism.

7. a) Explain the acidity of Cyclopentadiene and Cycloheptatriene.

    b) Explain briefly Claisen rearrangement.

8. a) Briefly explain Barton reaction.

b) Explain the photochemistry of olefins.

9. a) Discus the structure elucidation of Carotene.

b) Briefly describe the biosynthesis of terpenes.

10. a) Explain kinetic and thermodynamic control in reactions involving ketones.

b) Explain the reason for the difficulty in the hydrolysis of 2, 6 - disubstituted benzoic acid esters.

[5x5=25 marks]

SECTION-C

Answer **any three** questions and **each** question carries 10 marks.

11. i) Discuss the mechanism and applications of Beckmann rearrangement.

ii) Discuss the similarity in the intermediates of Curtius, Schmidt and Lossenrearrangements.

12 Explain briefly on

i) Sigmatropic reactions

ii) 1, 3 - Dipolar and Ene reactions.

13. Discuss the following:

i) Photochemistry of vision

ii) Photoreaction of Vitamin D.

14. Explain the following:

i) Structure of Estrone.

ii) Chemical, spectroscopic and chiroptical methods for establishing carbon skeleton.

15. Discuss the following:

i) Principles and applications of phase transfer catalysis.

ii) Methods of determination of reaction mechanism.   **[10x3=30 marks]**

Second Semester M.Sc. Degree Examination (Model Question Paper)

Branch: Medicinal Chemistry

CM 223/CH 223/CL 223/CA 223 : Physical Chemistry- II

(2016 Admission Onwards)

Time : 3 Hours   **Max mark : 75**

Section A

Answer any two among **(a)**, **(b)** and **(c)** from each question. **Each** sub-division carries **2** marks .

1. a) Set up the Schrodinger equation for a rigid rotator.

b) Give plots of (a) radial probability distribution functions of 2S orbital and (b) angular plot of $2P_x$ orbital.

c) Write the expression for fock operator and explain the terms

2. a) What are overtones? Why are they weak?

b) State and explain the rule of mutual exclusion with one example.

c) State Franck-Condon principle.

3. a) Explain the terms 'Force' and 'Flux' with reference to irreversible thermodynamics.

   b) Show the influence of temperature on the miscibility curve in a three component system forming a pair of partially miscible liquids.

   c) What are the conditions under which linear relations are valid to understand irreversible processes.

4. a) Derive ideal gas law from translational partition function.

   b) Explain the term canonical ensemble.

   c) Electron would never follow Maxwell Boltzmann statistics. Why?

5. a) What is Lippmann potential? How does it arise?

   b) Calculate the mean activity coefficient of $0.01M$ $BaCl_2$ in water at $25^{\circ}C$.

   c) Explain the origin of concentration overpotential. **(10 X 2 = 20 Marks)**

Section- B

Answer either **(a)** or **(b)** of each question and each question carries **5** marks

6. a) Explain self-consistent field method to solve many electron systems.

   b) Write the Schrodinger equation for hydrogen atom in polar coordinates and separate the variables.

7. a) Explain the principle and application of Laser Raman Spectrum.

   b) Explain the origin of P and R branches in rotational-vibrational spectrum.

8. a) Derive generalized equation for entropy production from heat flow.

   b) Give the Onsagar-reciprocal relations. What are its applications?

9. a) Apply Fermi-Dirac statistics to understand paramagnetism in solids.

   b) Derive the expression for partition function for particle executing (i) free linear motion and (ii) free linear harmonic vibration.

10. a) Derive Debye-Huckel limiting law.

    b) Discuss the various models for electrical double layer.

    (5 X 5 = 25 Marks)

Section-C

Answer **any three** questions and **each** question carries **10** marks

11. (i) Apply Schrodinger equation for particle in a ring. Find eigen values and eigen functions.

    (ii) Show that any two associated Legendre functions satisfy orthonormality condition.

12. (i) Give an account of rotation spectra of diatomic molecules. Explain the effect of nonrigidity of the bond on the spectra.

    (ii) How is the rotational spectrum of a diatomic molecule affected by isotopic substitution?

13. (i) Draw the phase diagram of a three component liquid system with three pairs of partially miscible liquids. Explain.

    (ii) How would you understand (a) thermo osmosis and (b) thermal diffusion from irreversible thermodynamics?

14. Derive the expression for the distribution function of a Boson and Bose-Einstein condensation.

15. (i) Derive Butler-Volmer equation. Deduce the expression for the low and high field limits of this equation.

    (ii) Discuss the application of Debye-Huckel Onsagar equation as applied to strong electrolytes and point out its limitations.

    (10 x 3 = 30Marks)

SEMESTER III

CM 231 INORGANIC CHEMISTRY- III

Total 90 h

Unit I Organometallic compounds
18h

Nomenclature of organometallic compounds. Hapto nomenclature. 18 and 16 electron rule, isoelectronic and isolobal analogy. Types of metal complexes. Metal carbonyls, bonding in metal carbonyls. Bonding in metal nitrosyls and cyanides. Synthesis, structure and bonding of polynuclear carbonyls with and without bridging. Complexes with linear π donor ligands: Olefins, acetylenes, dienes and allyl complexes. Complexes with cyclic π donors: Cyclopentadiene, benzene complexes, structure and bonding of ferrocene and dibenzenechromium complexes (MO treatment). Oxidative addition and reductive elimination, insertion and elimination reactions Catalysis by organometallic compounds: Alkene hydrogenation using Wilkinson's catalyst, hydroformylation of olefins using cobalt catalyst and polymerization reaction by Ziegler-Natta catalyst. Fluxional molecules.

Unit II Coordination chemistry-III: Reactions of metal complexes
18 h

Energy profile of a reaction - Thermodynamic and kinetic stability, Stability of complex ions in aqueous solutions: Formation constants. Stepwise and overall formation constants. Factors affecting stability of complexes. Determination of stability constants: spectrophotometric, polarographic and potentiometric methods. Stability of chelates. Thermodynamic explanation, macrocyclic effects. Classification of ligand substitution reactions -kinetics and mechanism of ligand substitution reactions in square planar complexes, trans effect-theory and synthetic applications. Kinetics and mechanism of octahedral substitution- water exchange, dissociative mechanism, associative mechanism- Eigen-Wilkins mechanism, Eigen-Fuoss equation, base hydrolysis, racemisation and isomerisation reactions. Electron transfer reactions: Outer sphere mechanism-Marcus theory, inner sphere mechanism- Taube mechanism. Photochemical reactions- substitution and redox reactions of Cr(III) , Ru(II) , and Ru(III) complexes. Photo-isomerisation and photo-aquation reactions of metal complexes.

Unit III Bioinorganic chemistry
18 h

Essential and trace elements in biological systems, structure and functions of biological membranes, mechanism of ion transport across membranes, sodium-potassium pump. Photosynthesis, porphyrin ring system, chlorophyll, PS I and PS II. Synthetic model for photosynthesis. Role of calcium in biological systems. Oxygen carriers and oxygen transport proteins- haemoglobin and myoglobin. Non-haeme iron-sulphur proteins involved in electron transfer-ferredoxin and rubredoxin. Iron storage and transport in biological systems-ferritin and transferrin. Redox metalloenzymes-cytochromes, peroxidases and superoxide dismutase and catalases. Nonredox metalloenzymes- CarboxypeptidaseA- structure and functions. Nitrogeases, biological nitrogen fixation. Vitamin B_{12} and coenzymes. Toxic effects of metals(Cd, Hg, Cr and Pb).

Unit IV Spectroscopic Methods in Inorganic Chemistry
18 h

Infrared spectra of coordination compounds. Structural elucidation of coordination compounds containing the following molecules/ ions as ligands- NH_3, H_2O, CO, NO, OH^- , $SO4^{2-}$, CN^- , SCN^- , NO_3^- , NO_2^- CH_3COO^- and X^- (X= halogen). Changes in ligand vibration on coordination with metal ions. Vibrational spectra of metal carbonyls- CD and ORD spectra of metal complexes. ESR spectra : Application to Cu(II) complexes and inorganic free radicals such as PH_4, F_2^- and $[BH_3]^-$. Nuclear Magnetic Resonance Spectroscopy :The contact and pseudocontact shifts, some applications including biological systems, an overview of NMR of metal nuclides with emphasis on $_{31}P$ and $_{19}F$ NMR. Mossbauer Spectroscopy : Application of the technique to the studies of iron and tin complexes.

Unit IV Nuclear chemistry
18 h

Nuclear structure, mass and charge. Nuclear moments. Binding energy. Semiempirical mass equation. Stability rules. Magic numbers. Nuclear models: Shell, Liquid drop, Fermi gas, collective and optical models.

Equation of radioactive decay and growth. Half life and average life. Radioactive equilibrium. Transient and secular equilibria. Nuclear reactions: Direct nuclear reactions, heavy ion induced nuclear reactions, photonuclear reactions. Neutron captures cross section and critical size. Nuclear fission as a source of energy, Nuclear chain reacting systems. Principle of working of the reactors of nuclear power plants. Breeder reactor. Nuclear fusion reaction, stellar energy.   Principles of counting technique such as G.M. counter, proportional, ionization and scintillation counters. Cloud chamber.

References

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2.   J. E. Huheey, Inorganic Chemistry-Principles of Structure and Reactivity, Harper and Collins, 4th edition, 2011.

3.   E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock, Structural methods in Inorganic Chemistry, Blackwell, Oxford, 1987.

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5.   R.V. Parish, NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, Ellis Harwood, Chichester, UK 1999.

6.   G. Friedlander and J. W. Kennady, Introduction to Radio chemistry, John Wiley and Sons New York, 1949.

7.   H. J. Arnikar, Essentials of Nuclear Chemistry, New Age International, New Delhi, 4th edition, 1995.

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9.   R. W. Hay, Bioinorganic Chemistry, Ellis Horwood, Chichester, 1987.

10.   P. Powell, Principles of Organometallic Chemistry, Chapman and Hall, 2nd Edition, New York, 1988.

11.   S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, Mill Valley, California, 1994.

12.   D. E. Fenton, Biocoordination Chemistry, Oxford University Press, Oxford, 1995.

13.   R. C. Mehrothra and A. Singh, Organometallic Chemistry: A Unified Approach, Wiley eastern, 1991.

14.   D. F. Shriver, P. W. Atkins and C. H. Langford, Inorganic Chemistry, ELBS, Oxford University Press, 1990.

15.   L. Bertin, H.B. Gray, S. J. lippard and J. S. Valentine, Bioinorganic Chemistry, Viva Books Pvt. Ltd, New Delhi, 1998.

CM232 ORGANIC CHEMISTRY-III

Total 90 h

Unit I UV-Vis and IR Spectroscopy and Mass spectrometry   18h

Electronic transitions and analysis of UV spectra of enes, enones and arenes. Woodward-Fieser rules. Effect of solvent polarity on UV absorption. Principle of characteristic group frequency in IR. Identification of functional groups and other structural features by IR, Hydrogen bonding and IR bands. Sampling techniques. Mass spectrometry- EI, CI, FAB, Electrospray and MALDI ion sources. Magnetic, High resolution

(Double focusing), TOF and quadrupole mass analysers.Characteristic EIMS fragmentation modes and MS rearrangements. Mass spectral fragmentation patterns of long chain alkanes, alkenes, alkynes, alcohols, ethers, thiols, aromatic compounds, aldehydes, ketones, acids, amides, nitro, amino and halo compounds.

Unit II NMR spectroscopy and structural elucidation18h

Theory of NMR spectroscopy, chemical shifts, anisotropic effects and coupling constant.Spin-spin interactions in typical systems. First order and higher order spectra. Simplification methods of complex spectra by high field NMR, shift reagents, chemical exchange and double resonance. ^{13}C NMR chemical shifts. Applications ofNOE, DEPT, and 2Dtechniques such as COSY, HSQC, HMQC and HMBC. Spectral interpretation and structural elucidation. Solving of structural problems on the basis of numerical and spectrum based data.

Unit III Organic synthesis18 h

C-C and C=C bond forming reactions. Mannich, Reimer-Tiemann, Synthesis of small rings.Simmons-Smith, Vilsmeier-Haack, Ullmann and Chichibabin reactions. Ring formation by Dieckmann, Kostanecki, Thorpe, Pschorr and acyloin condensations. Stork enamine, Shapiro, Peterson, Heck, Stille, Ritter and Prilezhaev reactions.Reduction and oxidation in synthesis.Catalytic hydrogenation.Alkali metal reduction, Birch reduction, Clemmensen reduction and Wolff-Kishner reduction, Huang-Minlon modification.Boranes,LAH and sodiumborohydride as reductants.Hydrogenation, Oppenauer oxidation, Jones oxidation.Applications of HIO_4, OsO_4 and mCPBA.Organo palladium catalysts -Heck, Negishi, Sonagashiraand Suzuki coupling

Unit IV Methods in organic synthesis18 h

Retrosynthetic analysis and disconnection approach. Synthetic strategy and synthons.Regioselectivity in enol and enamine alkylation.Stereospecific and steroselective synthesis, Sharpless asymmetric epoxidation, Chiral pool, chiral auxiliary, Chiral reagents, BINAP, Mitsunobu reaction. 1,3-dipolar cycloaddition in the construction of rings. Olefin synthesis by extrusion reactions.Olefin metathesis – first and second generation Grubbs' catalysts.Umpolung concept, functional group equivalents.Reductive coupling reactions.Epoxide to alkene.Introduction to combinatorial synthesis.Electrochemical reduction of organohalogen, nitro and carbonyl compounds.Electrochemical Kolbe oxidation.Protecting group strategy: Tetrahydropyranyl, silyl, *t*-butyl, trichloroethyl, acetal and thioacetal as hydroxyl, thiol, carboxyl and carbonyl protecting groups in synthesis.

Unit V Separation techniques18 h

Classification of chromatographic methods.Theory of chromatography.Applications of chromatographic methods.Adsorption and partition chromatography.Paper, thin layer and column chromatographic methods.Centrifugal TLC, LC, Pressure column chromatography, HPLC and GC.Column matrices.Detectors.Affinity and chiral separations using HPLC.Normal and ultra-centrifugation.Gel and Capillary electrophoresis and their applications.Solvent extraction.Extraction using supercritical liquid CO_2, Craig's technique of liquid-liquid extraction.

References

1.	D. H. Williams and I. Fleming, "Spectroscopic methods in organic chemistry," 6thEdition, Tata McGraw Hill, 2011

2.	W. Kemp, "Organic spectroscopy,"3rd Edition, Palgrave Macmillan, 1991

3.	D. L. Pavia, G. M. Lampman, G. S. Kriz and J. A. Vyvyan, "Introduction to Spectroscopy," 4th Edition, Brooks Cole, 2008.

4.	S. N. Issacs, "Physical organic chemistry," Prentice Hall 2nd edition, 1996.

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6.	J. Hine, "Physical organic chemistry,"2nd Edition, McGraw-Hill, 1962

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8. H.O. House, "Modern synthetic reactions," 2nd Revised Edition, Benjamin Cummins, 1965.

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10. W.Carruthers, "Modern methods in organic synthesis," 3rd Edition, Cambridge University Press, 1987.

11. J. Singh and L. D. S. Yadav, "Organic Synthesis,"PragatiPrakashan, 2010.

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14. D. J. Holme and H. Perk, "Analytical Biochemistry," 3rd Edition, Prentice Hall, 1998.

CM 233 Physical Chemistry -III   **90 Hrs**

Unit I Chemical Bonding   **18 hrs**

Approximate methods: method of Variation - Variation theorem and its proof. Linear variation functions. Secular equations and secular determinants.Perturbation method-Successive correction to an unperturbed problem. Detailed treatment of first order non-degenerate case only.

Treatment of molecules- The Born- Oppenheimer approximation- LCAO-MO Theory- MO theory of H_2 and H_2^+. MO treatment of other homo diatomicmolecules Li_2, Be_2, B_2, C_2, O_2 and F_2. MO treatment of hetero diatomic molecules LiH,CO, NO and HF. Spectroscopic term symbols for homo diatomic molecules.

Valance bond theory of diatomic molecules H_2 O_2 and F_2. Comparison of MO and VB theories, Quantum mechanical treatment of SP, SP^2 and SP^3Hybridisation.HMO theory of conjugated systems. Bond order and charge density calculations,Free valance.Application of HMO method to ethylene, allyl system, butadiene and benzene.

Unit II Computational Chemistry   **18 hrs**

Introduction to computational chemistry : as a tool and its scope. Potential energy surface- stationary point, saddle point or transition state, local and global minima.Slater and Guassian functions and its properties. **Basis sets** : minimal, double zeta, triple zeta basis sets, contracted basis sets, Pople's style basis sets and their nomenclature.Basis functions- Roothan's concept, Slater type orbitals (STO) and Gaussian type orbitals (GTO).Slater determinants

Quantum mechanical computational methods-Ab initio methods: Introduction to SCF. Wave functions for open shell state, RHF, ROHF and URHF. (no calculation). Electron correlation and introduction to post HF methods.

Semiempirical methods. Huckels and extended Huckel methods. Strengths and weaknesses. PPP, ZDO and CNDO approach. (Mentioning only).

Density functional theory- Hohenberg-Kohn theorems, Exchange co-relational functional.(Only the basic principles and terms to be introduced).

Non-quantum mechanical computational methods-Molecular mechanics: Force fields, bond stretching, angle bending, torsional terms, non-bonded interactions, electrostatic interactions and the corresponding mathematical expressions. Names of some commonly used force fields.

Construction of Z-matrix for simple molecules. H_2O, H_2O_2, H_2CO, CH_3CHO, NH_3 and CO_2.

Unit III Spectroscopy II   18 hrs

Resonance spectroscopy: Nuclear Magnetic resonance Spectroscopy, Nuclear spin.Interaction between nuclear spin and applied magnetic field. Proton NMR . Population of energy levels. Nuclear resonance. Chemical shift. Relaxation methods. Spin-spin coupling.Fine structure. Elementary idea of 2D and 3D NMR. Introduction to instrumentation.

ESR spectroscopy: Electron spin. Interaction with magnetic field. Kramer's rule. The g factor. Determination of g values. Fine structure and hyperfine structure. Elementary idea of ENDOR and ELDOR.

Mossbauer spectroscopy: Basic principles. Doppler effect, chemical shift, recording of spectrum, application. Quadrupole effect.

NQR spectroscopy - Principle and application

Photoelectron spectroscopy. Introduction to UV photoelectron and X-ray photoelectron spectroscopy.

Unit IV Statistical Mechanics II   18 hrs

Molecular partition functions. Translational (1D, 2D and 3D), vibrational, rotational and electronic partition functions. Total partition functions Langevin function and its use for the determination of dipole moment.and molecular energies

Relation ship between Partition functions and thermodynamic properties, The principle of equipartition of energy. Chemical equilibrium. Law of mass action. Transformation of the equilibrium expressions. Statistical derivation.Thermodynamic probability and entropy.

Equipartition principle Quantum theory of heat capacity. Calculation of heat capacity of gases, limitation of the method. Heat capacity of solids. Dulong and Petit's law, Kopp's law, Classical theory and its limitation. The vibrational properties of solids. Einstein theory of heat capacity. The spectrum of normal modes. Limitations of Einstein's theory. The Debye theory, the electronic specificheat.

Unit V Electro Analytical and Spectrophotometric methods.   18 hrs

Potentiometric methods: Reference electrodes and indicator electrodes. The hydrogen,calomel, Ag-AgCl electrode. The glass electrode- its structure, performance and limitations.Measurement of pH. Potentiometric titrations- redox and precipitation titrations.

Electrogravimetry: Principle and method. Determination of Copper. Separation of metal ions.

Conductometry: Principle and method. Conductometric titrations.

Coulometry: Principle andmethod. Coulometric titrations.

Voltametry: principle and method of polarography, cyclicvoltammetry, stripping voltammetry and amperometry.

Flame emission and atomic absorption spectrometry. Instrumentation for AAS. The flame characteristics. Atomiser used in spectroscopy. Hollow cathode lamp. Interference in AAS. Application of AAS.

References

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7. J.P Lowe, K. Peterson, "Quantum Chemistry", New Age International

8. E. Lewars, "Computational Chemistry- Introduction to the Theory and Applications of Molecular and Quantum Mechanics", Springer.

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15. L.K.Nash, "Elements of Statistical Thermodynamics", Addison Wesley Publishing Co.

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19. B.Widom, Statistical Mechanics – A concise Introduction for Chemists. Cambridge University Press.

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21. D.A.Skoog, D.M.West and F.J.Holler," Fundamentals of Analytical Chemistry" Saunders College.

22. Puri, Sharma, Pathania,"Principles opf physical Chemistry"Vishal publishing company.

23. Gurdeep Raj "Advanced Physical Chemistry" GOEL Publishing House, Meerut.

24. F.W. Sears and G.L. Sailinger" Thermodynamics, Kinetic Theory, and Statistical Thermodynamics" Third edition. Narosa publishing House , New Delhi.

CM 234 Quantitative Organic Practical   125hrs

A. **Estimation and extraction of medicinal compounds**

I. Organic Estimations

1. Estimation of Carbohydrates

2. Estimation of Nucleic acids

3. Estimation of Proteins

4. Estimation of Lipids

5. Estimation of Amino acids

6. Estimation of Vitamins

B. Extraction of natural products

1. Soxhlet extraction of the alkaloids from any plant.

C. Chromatographic Analysis:

1. Analysis of amino acids by thin layer chromatography or paper phromatography.

2. Paper chromatography of carbohydrates.

3. Column Chromatography for enzyme protein analysis.

4. Drug analysis: Paracetamol,Aspirin, Benzyl benzoate, etc.

5. Study of UV absorption spectra of macromolecules (protein and nucleic acid).

D. Spectral identification

(UV,IR,1H NMR,C13 NMR,EI mass) of organic compounds from a library of organic compounds.

35

References:

1.   Fundamental of Analytical Chemistry, Skoog&West, Holt,Rinehart and Winston.

2.   Chromatography: Concepts and Contrasts- 1988 by James Miller. John Wiley and Sons.

3.   Spectroscopy, Volume 1.Edited by B.B. Straughan and S. Walker.Chapman and Hall.

4.   Instrumental Methods of Analysis. 6th Edition by H.H. Willard, L.L. Merritt Jr. *et. al.*1986. CBS Publishers and Distributors.

5.   Phytochemical Methods: A Guide to Modern Techniques of Plant Analysis,3rd Edition, J.B. Harborne, Chapman and Hall,London, 1998.

6.   Experimental Phytochemical Techniques, N. Raaman, New India Publishing Agency, New Delhi, 2011.

7.   F.G.Mann and B.C.Saunders, "Practical Organic Chemistry", Longman.

CM 235 Computational Techniques Lab-I   125hrs

A. Basic programming

1.   Basic UNIX commands, shell scripts and the first C-programming.

2.   Algorithm, flowchart,basic data types and control structures in C++.

3.   Managing classes and objects in a variety of situations.

4.   Solving moderately complex problems involving the above and requiring selection of appropriate structures and algorithms.

5.   PDB and graphics visualization, basics of visualizing molecules using Pymol,Chimera, Sequence analysis at Expasy and PDB.

6.   Protein Crystallization: Preparation of different forms of Lysozymecrystals with different conditions.

7. Visualizing reciprocal lattice and diffraction through Ewald sphere using X-Ray View.

8. X-ray diffraction and data collection (When X-ray in house source is available).

9. Molecular Replacement: Using AMoRestand alone package express mode and less automated mode.

B. Chemical databases

1.   ChemBank
2.   ChemBio Finder
3.   CS Chemoffice
4.   ZINC data base
5.   Dr Dukes phyto chemical database
6.   Pubchem data base
7.   BIDD
8.   OSDD CHEM

C. Molecular dynamics: NWChem /GAMESS free / Hyperchem /Guassian / Jaguer Macro model. Energy calculation and minimization.

1. Calculate the current energy of a compound in gas phase and minimization of energy in gas phase and report the energy of particular molecule?

2. Calculate the current energy in solution phase and minimization of energy and report the energy of particular molecule.

3. Calculate the minimization energy of given substructure 5a° apart from Ligand and the residues by keeping 10a°-15a°atom frozen.

4. Calculation of molecular orbital of given molecule.

5. Calculations of electronic properties of proteins.

6. Calculation of geometrical parameters of molecule by applying periodic boundary condition.

7. Calculate the IR frequency of the given compounds and compare with the Given experimental data.H_2O,CH_4,C_2H_6,C_2H_5OH,CH_3COCH_3,CH_3CHO,parcetamol, aspirin.Using methods: HF,B3LYP.Basis set:6.31G*,6-31+G*

8. Calculate the structural parameters of a given molecule after dynamic simulated annealing and geometry optimization.

9. Comparison of heat of formation of different molecules (halogen acids by semi-emprical (PM3)).

10. Calculate the vibration in IR spectra due to hydrogen bonding in acetic acid dimmers and compare IR spectra and structural parameters with monomer data.

11. Compare the molecular energy parameters of 6th group hydrides and compare with experimental data.

12. Predict the proton affinity of pyridine by PM3 and AM1 methods.

13. Calculate the charge distribution and depict pi molecular orbitals in various substituted benzenes.

14. Compare the geometrical and spectrochemical parameters of acetic acid by using ab-initio and semi-empirical methods.

15. Calculate the spectroscopic and geometrical parameters of ethyl alcohol using ab-initio, semi-empirical and molecular mechanics methods.

References:

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2. Argus lab/ Schrodinger manual.
3. Introduction to Computational Chemistry -Frank Jensen [wiley Publications]
4. Deitel & Deital, C++: How to Program, Pearson Education, ISBN 81-297-0276-2
5. Deitel N M, C++: How to Program, Lab Manual, ISBN 0-131-4099-9
6. **www.cplusplus.com**
7. Computational Chemistry: A Practical Guide for Applying Techniques in Real-Worlds Problems David C. Young Wiley Interscience A John Wiley & Sons.INC. Publication.

CM 236 Computational Techniques Lab-II   125hrs

A. Medicinal chemistry (GOLD/Glide/ Sybyl / Vlife/Auto Dock, Power MV, Open Babel,Cygwin)

1. Docking
2. Protein preparation.
3. Ligand preparation.

4. Active site determination.

5. Docking.

6. ADMET prediction.

7. Dataminig (WEKA)

a. Development of QSAR model by using the given experimental data and its validation.

b. Building of predictive models for given targets by using various data mining techniques.

B. Computer programming
Perl

1. Setting up Perl Development Environment.

2. Perl Program.

3. Perl Scalar Variables.

4. Perl If Control Structure.

5. Perl For Loop Statement.

6. Perl While Loop.

7. Perl Array.

8. Perl Hash.

9. Perl Subroutine.

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2. Schrodinger manual .

3. Argus lab manual.

4. Hyperchem manual.

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Third Semester M.Sc. Degree Examination – Model question paper

Branch – Medicinal Chemistry

CM/CH/CL/CA 231 : INORGANIC CHEMISTRY- III

(2016 Admission Onwards)

Time : 3 Hrs   Max. Marks: 75

SECTION A

Answer **two** among **(a), (b)** and **(c)** from **each** question carries **2** marks

1. a) Draw the structure of $Rh_4(CO)_2$.
   b) How do sigma allyl complexes differ from pi allyl complexes?
   c) What are fluxional molecules?

2. a) What are the factors affecting the stability of complexes?
   b) Explain Macrocyclic effect?
   c) What is anation reaction? Give an example.

3. a) Why electron transfer process in photosynthesis is called an uphill process?
   b) Explain the mechanism of oxygen binding in haemocyanin.
   c) What is Na^+ - K^+ pump? How does it function?

4. a) What is group frequency concept? Illustrate with example.

   b) Why are solid samples used for recording Mossbauer spectra?

   c) What is Dopplar broadening? Explain with an example.

5. a) Explain binding energy.

   b) What is compound nucleus? How is it formed?

   c) Give a note on breeder reactors. **(2x10= 20 marks)**

SECTION B

Answer either among **(a) or (b)** from **each** question carries **5** marks

6. a) What are metal carbonyls? Explain the structure and bonding in $Ni(CO)_4$

   b) Discuss the mechanism of polymerization of Zeigler- Natta catalyst.

7. a) Explain Trans effect with suitable examples.

   b) Give an account of photochemical reactions of complexes.

8. a) Discuss the role of calcium in blood clotting process.

   b) Explain the structural features of haemoglobin.

9. a) How does IR spectroscopy help for the structural elucidation of complexes containing ammonia and water as ligands.

   b) Explain CD and ORD spectra of complexes.

10. a) Distinguish between Transient and Secular equilibria.

    b) What is meant by half life period? How is it related to decay constant? The $t_{1/2}$ of a radio nuclide is 20 years. If a sample of this nuclide has an initial activity of 8000 disintegrations per minute today, what will be its activity after 80 years?

    (5x5= 25 marks)

SECTION C

Answer **any three** questions. **Each** question carries **10** marks

11. Explain the bonding of ferrocene by MO Theory.

12. Briefly explain outer sphere and inner sphere mechanism of electron transfer reactions

13. i) Discuss the function of PS-I and PS-II in photosynthetic activity.

    ii) Outline the probable mechanistic pathways Nitrogenase activity in nitrogen fixation.

14. i) Discuss the application of ESR spectroscopy to Cu(II) complexes.

    ii) Explain how Mossbauer spectroscopy helps to the studies of iron and tin complexes

15. Discuss about different types of nuclear reactions with suitable examples.

    (10x3= 30 marks)

THIRD SEMESTER M.Sc.DEGREE EXAMINATION

BRANCH – MEDICINAL CHEMISTRY

CH/CL/CA/CM 232: Organic Chemistry-III

(2016 admissiononwards)

Time-3 hours   Maximum marks :75
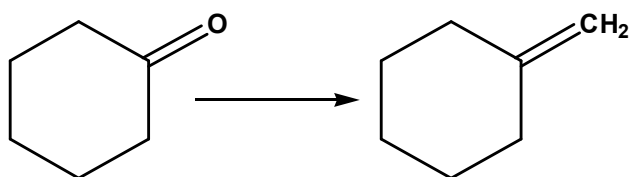
Section A

Answer any two among (a), (b) and (c) from each question.

Each sub question carries 2 marks

1   a) Explain how CH stretching vibrations of sp, sp^2, sp^3 hybridised carbon varies.

b) Polar solvents usually produces a red shift in the $\pi' \to \pi$ transition explain.

c) Explain how the presence of bromine atom in a molecule can be detected by mass spectrum.

2   a) Explain why acetylenic hydrogens are more upfield than vinylic hydrogens.

b) What multiplicities are observed for the signals of off resonance decoupled ^{13}C spectrum of 2-chloropropene?

c) Account for the fact that splitting is observed between Hydrogens "a" and b in 2-methyl propene $(CH^a_3)_2C=CH^b_2$ and not in neo pentylchloride $(CH^a_3)_3CH^b_2\,Cl$.
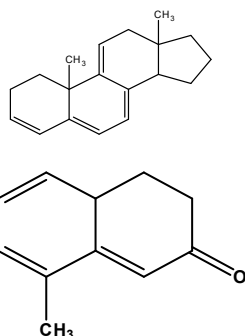
3   a) Suggest a method for conversion

b) What is Clemmensonreduction

c) What are enamines? Write one synthetic application of enamine

4   a) Explain the use of silyl group as protecting group in organic synthesis.

b) Explain the term combinatorial synthesis

c) What is umpolung?

5   a) What is the principle of chromatography

b) What is paper chromatography? How is it helpful in identifying various alpha amino acids?

c) Outline the applications of Gel electrophoresis.   **(2x10= 20 marks)**

Section B
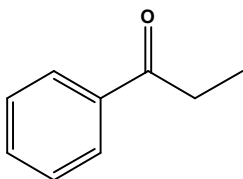
Answer either (a) or (b) from each question. Each sub question carries 5 marks

6   a) By using Woodward Fieser rules calculate the ë max values
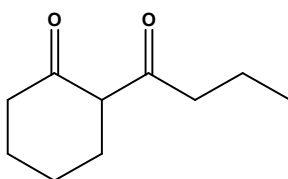

b) How IR spectrum can be used to distinguish

i) Primary amine from primary amide   ii)) Ethyl benzene from o-xylene

7   a) Deduce the identity of the compound $C_9H_{10}O$ that has an IR absorption at 1688 cm-1 and 1 H NMR signals at 1.22 (triplet, 3 H), 2.98 (quartet) and 7.28-7.95 (multiplet, 5H).Assign the data

   b)   Explain the paramagnetic anisotropy of alkenic, aldehydic and aromatic protons.

8   a)   Discuss Vilmeier-Hack reaction.
     b)   Write short notes on important metal hydrides used as reducing agents in organic synthesis

9   a)   Explain the regioselective synthesis of the following compound from cyclohexanone

   b)   Discuss the synthesis of β-hydroxy ketones and aldehydes usingumpolung

10   a)   Explain the principle of gas chromatography and ion exchange chromatography. What type of substances are analysed using the above?
     b)   Describe the principle and instrumentation of HPLC   **(5x5= 25 marks)**

Section C

Answer any three questions.Each question carries 10 marks

11.   Discuss the functional group and finger print regions in the IR spectrum. How the IR spectrum is useful in distinguishing the inter and intra molecular hydrogen bonding

12.   Write short notes on
      i) DEPT spectra, ii) Nuclear Overhauser effect, iii) Shift reagents in NMR,
      iv) Double resonance NMR

13.   Explain the following named reactions with mechanism and example
      i) Mannich reactions ii) Robinson annulations reactions iii) Suzuki coupling

14.   Explain olefin metathesis and Mitsonubu reaction with applications of each

15.   With a schematic diagram explain the principle, instrumentation, and applications of GC
                                                            (10x3= 30 marks)

THIRD SEMESTER M Sc. CHEMISTRY DEGREE EXAMINATION
BRANCH – MEDICINAL CHEMISTRY
CH/CL/CA/CM 233 – Physical Chemistry III
(2016 admission ownwards.)

Time : 3 Hours   Max. Marks : 75

Section A

Answer any two among (a), (b) and (c) from each question.
Each sub question carries 2 marks

1)   A) Arrange O_2, O_2^+, O_2^- in the increasing order of stability. Justify your answer

B) Write briefly about "Perturbation theory"

C) Explain the more dipole moment in ethyl chloride than in chlorobenzene.

2)   A) Construct the z-matrix of CH_3CHO.

B) Name any two chemistry related software.

C) Write the determinantal wavefunction for the configuration $1S_2 2Pz$

3)   A) Write the expression for chemical shift in Mossbauer spectroscopy and explain the terms.

B) Calculate the ESR frequency of an unpaired electron in a magnetic field 0.33 Tesla. Given for free electron g=2, â=9.273×10^{-27} J/T

C) Explain the basic principle of X-ray photoelectron spectroscopy.

4)   A) Calculate the value of $\ln 6\tilde{A}$ with and without Stirling's theorem. Find the difference between the values if any. Comment on the result.

B) What is meant by the law of equipartition of energy?

C) State and explain Dulong Petit's law. Explain its limitations.

5)   A) What are the requirements for choosing a reference electrode?

B) Define half wave potential. Explain its significance.

C) Why do we use three electrodes in cyclic voltametry.

(2x10= 20 marks)

Section B

Answer either (a) or (b) from each question. Each sub question carries 5 marks

6)   A) Derive the expression for the bond angle and wave function in sp^2 hybridisation.

B) Apply HMO theory to butadiene molecule and discuss the molecular orbitals and their corresponding energy levels.

7)   A) Differentiate between Slater type orbitals and Gaussian type orbitals

B) What is potential energy surface? Explain its significance.

8)   A) Write a brief account of 2D-NMR spectroscopy.

B) What is Kramer's degeneracy? Discuss.

9)   A) B) Give comparison between Bose-Einstein, Maxwell-Boltzmann and Fermi-Dirac statistics.

B) Explain briefly how heat capacity of gases can be calculated?

10)   A) Explain the working of glass electrode.

B) Discuss the advantages and disadvantages of amperometric titrations.

(5x5= 25 marks)

Section C

Answer any three questions. Each question carries 10 marks

11)   Write a note on the secular equations.

12)   Discuss Density functional theory and give its advantages and limitations.

13)   Explain the principle and applications of NQR spectroscopy.

14)   Derive Einstein's heat capacity equation for solid.

15)   Describe the theory and instrumentation of AAS.   **(10x3= 30 marks)**

SEMESTER IV

CM:241 INTRODUCTORY COURSE IN MEDICINAL CHEMISTRY

Unit I Basics of Cheminformatics and Bioinformatics   18hrs

History of scientific information communication, chemical literature, chemical information, chemical information search, chemical information sources, chemical name and formula searching, analytical chemistry, chemical history, biography, directories and industry sources. Introduction to cheminformatics: History and evolution of cheminformatics, use of cheminformatics, prospects of cheminformatics. Representation and manipulation of 2D and 3D molecular structures, molecular descriptor technology, calculation of physical & chemical data, calculation of charge distribution Introduction to bioinformatics: Experimental sources of biological data, publicly available databases, gene expression monitoring, genomics and proteomics, metabolomics, visualisation of sequence data, visualization of structures using Rasmol or SPDB Viewer or CHIME.

Proteine structure prediction: Protein identification & characterization, primary structure analysis & prediction, secondary structure analysis & prediction, methods, abinitio approach for protein prediction, protein prediction from DNA sequence.Conformational analysis:conformational space-methods,model building approaches,random search methods,distance geometry,its use in NMR. Applications of bioinformatics in the field of medicine.

UNIT II - Basics of Medicinal Chemistry   18hrs

Definition, historical evolution, fundamental aspects of drug, classification of drugs,nomenclature of drugs, rules for nomenclatures. Genesis of drug (serendipity) random screening, molecular modifications, theoretical aspects of drug actions. Psycho pharmacological agents: Central nervous system depressants, central nervous system stimulant. Pharmacodynamic agents: Mechanism of action of peripheral nervous system drugs, histamines and anti-histamines cardiovascular drugs, locally acting drugs.Drugs for metabolic diseases and endocrine functions, drugs for metabolism and nutrition, water and mineral metabolism drugs and their mechanism of action.

UNIT III - Molecular basis of drug action: Receptor: 18hrs

Drug Receptor Interaction: Basic concept of ligand, agonist, antagonist, partial agonist, inverse agonist, receptor theories - occupancy, rate & activation theories, receptor binding assays, determination of B-max and Kd by transforming data with hill plot and scatchard plot, above concepts with special reference to opioid, adrenergic and GABA nergic receptors, GPCRS receptors . Enzyme Inhibition: enzyme, enzyme kinetics, enzyme inhibitors - reversible, irreversible, Kcat inhibitors.Transition state analogs, enzyme inhibitors as drugs - ACE, cycloxygenase, DNA polymerase inhibitors, HIV - protease/reverse transcriptase and cytochrome P-450 inhibitors. Basic idea about the drug binding to nucleic acid: anti-malarial & anti-cancer drugs.

Unit IV Molecular Dynamics & Protein Folding   18hrs

Molecular Dynamics: Idea about classical method, Langevin method, QM method. Molecular Dynamics using simple models. Dynamics with continuous potentials.Constant temperature and pressure dynamics, constraint dynamics. Conformation searching, Systematic search. Applications to protein folding. Comparative protein modelling: Modelling by Homology-the alignment, construction of frame work, selecting variable regions, side chain placement and refinement, validation of protein models Ramchandran plot, threading and ab initio model.

UNIT V GRAPH THEORY ,STATISTICS AND CHEMOMETRICS   18h

Graph theory and molecular numerology: basics of graph theory, matrix representations, adjacent matrix, distance matrix, atom connectivity matrix, incidence matrix, bond matrix,connection table. Chi-square test, z-test, t-test, F-test, tests of significance: testing hypotheses, tests of significance based on normal distribution. Analysis of variance: 1-way, 2-way and 3-way classification. Mathematical reasoning, induction and recursion;

Counting; graphs, trees and sets, basic probability and statistics; Markov processes. Multiple regression, tests of significance: testing hypotheses, tests of significance based on normal distribution. Chemometrics, commercial & open softwares.

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12. A Gringuage, Introduction to Medicinal Chemistry, Wiley-VCH, 1997.

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25.   S.C. Gupta, V.K. Kapoor. Fundamentals of applied statistics, New Delhi: Sulttaan Chand and sons; 4th edn., 2007.

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CM: 242 ADVANCED COURSE IN MEDICINAL CHEMISTRY

UNIT 1 PHARACEUTICAL APPLICATIONS OF MOLECULAR MODELLING   18h

Pharmacophore design, modification of structure to increase potency, ligand-based design and *De Novo* drug design,general principles of *de novo design,* automated *de novo design,*various steps involved in automated *de novo design,*idea about the softwares used for this.

Gaussian Process Models,Kernel Methods and Support Vector Machines,Theorems for Gaussian Processes and SVMs Molecular Dynamics: Further Topics - Brownian Dynamics (BD), Brownian Motion ,Brownian Framework , Hydrodynamic Interactions, Data Compression Based on Principal Component Analysis (PCA)Hierarchical cluster analysis (HCA), scaffold hopping, Force Fields :Formulation of the Model and Energy ,Bond Length Potentials ,Bond Angle Potentials ,Torsional Potentials ,The van der Waals Potential, The Coulomb Potential, Parameterization ,Force Field Comparisons ,Force Field Performance.

UNIT 2 PHARMACOKINETICS AND PHARMACODYNAMICS   18 h

General classiûcation of pharmacokinetic properties ,Drug regimens ,The importance of pharmacokinetics in drug discovery ,Drug concentration analysis and its therapeutic signiûcance, Concept of pro-drug and soft drug.Pharmacokinetic models ,Intravascular administration ,Distribution ,Extravascular administration ,Dissolution ,Absorption ,Single oral dose ,The calculation of tmax and Cmax ,Repeated oral doses , The use of pharmacokinetics in drug design

Pharmacodynamics: Introduction, concept of drug receptors interactions. Theories of drug activity relationship, treatment of diseases by enzyme stimulation and enzyme inhibition, elementary treatment of drug receptor interaction, LD50, ED50, MIC and MEC.

Quantitative structure activity relationship: QSAR Parameters - Lipophilicity,electronic and steric factors. Quantitative Models – Hansch analysis, Free Wilson analysis, mixed approach, Structure-based drug design.QSAR and 3D-QSAR methods.QSAR with molecular field analysis (MFA) and comparative molecular field analysis (CoMFA).

UNIT 3 FRAGMENT BASED DRUG DISCOVERY   18h

The fragment based lead discovery, Development and evolution of fragment-based drug design.Pitfalls to finding fragments. Epitopes, Fragment evolution,Fragment self assembly,Click chemistry in situ. Overview of potential screening methods – advantages and disadvantages.Under standing linking rules and cleaving rules of fragments.The use of virtual fragment based screening,rule of three for fragment-based lead discovery, application of fragment based drug design for membrane proteins such as GPCRs. Challenges, and Applications of FBDD. Advantages of FBDD over high throughput screening. Fragment-based de novo drug design. GPCR ligands as drug targets,GPCR-ligand data.

Docking of ligands,manual docking,automatic docking,molecular surface of binding site,rigid docking by shape complimentarity,use of grid in docking programmes,rigid docking by matching hydrogen bonding groups.

UNIT 4 DATA MINING   18h

Neural networks, artificial neurons,models of neuron - McCulloch-Pitts model, neural networks and architectures introduction,single, multilayer, recurrent networks.Learning methods - supervised, unsupervised and reinforced learning,.Advanced neural network architectures, feed forward neural networks. Self organizing feature map introduction, applications of SOFM.

Cheminformatic tools in high throughput screening.HTPS by NMR, affinity screening, surface plasmon resonance(SPR), scintillation proximity assay(SPA),virtual screening.

Data Mining Tasks- Classification ,Clustering ,Association Summarization, Text Mining, Data Mining Techniques- Databases and Data Warehousing, Statistics, Graphical Models :Bayesian Networks Classiûers:Regression-Based Classiûers, Neural Network Classiûers, Some Observations about Linear Classiûers.

UNIT 5 ORGANIC MEDICINAL CHEMISTRY   18h

Drug metabolic reactions: Phase I (oxidation, reduction or hydrolysis), or Phase II (conjugation), factors affecting drug metabolism.

Important medicinal compounds: General Anesthetics, characteristic features of ideal general anaesthetics,mechanism of action of general anaesthetics,examples of general anaesthetics (trichloroethylene,thiopentone, ketamine) preparation and properties.

Sedative-hypnotic drugs: classification of sedative- hypnotic drugs, Barbiturates, chemistry of barbiturates, SAR of barbiturates , mechanism of action of barbiturates, examples of barbiturates drugs(Methaqualone, Chloral Hydrate (Trichloroacetaldehyde), Paraldehyde) npreparation and properties.

Therapeutic uses of natural products such as streptomycin, erythromycin, Study of the therapeutical efficacy of Laxatives:(aloe,senna), Cardiotonics:(digitalisarjuna), Anti-hypertensive: (rauwolfia),Anti-tumor: (vinca), Oxytocic: (ergot). Illustration of drug action through examples-Antibacterialsagents: Pencillin, mechanism of antibacterial action & SAR. Anticancer agents:Taxol - mechanism of action & uses. Antidiabetics: Diasulin mechanism of action & application. Anticholestemics: Mevastatin origin & mechanism of action.

Reference

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CH 243 DISSERTATION

Instructions to Question Papers Setters

The Syllabus of each theory has five units. While setting the question papers, equal weight is to be given to each of the Units for choosing the questions. Each question paper is of 3 hours duration and has three Sections, namely Section A, Section B and Section C constituting a total 75 marks as detailed.

Section A Five questions, one from each Unit containing three short answer questions marked (a), (b), and (c), each of which has 2 marks. One has to answer any two of (a), (b) or (c) from each of the five questions. (2x10=20 marks)

Section B Five questions, one from each unit containing two short essay questions marked

(a) and (b), each of which has marks. One has to answer either (a) or (b) from each of the five questions.   (5x5=25 marks)

Section C Five essay questions, one from each unit having 10 marks. One has to answer any three questions from the five questions asked.(10x3=30 marks)

Structures should be in chemdraw or ISIS/ draw

FOURTH SEMESTER M.Sc. DEGREE EXAMINATION

Branch : MEDICINAL CHEMISTRY

(Under Semester System w.e.f 2016 Admissions)

CM :241 INTRODUCTORY COURSE IN MEDICINAL CHEMISTRY

Time: 3 Hours   Maximum marks: 75

Section A

Answer any two among (a), (b) and (c) from each question. Each sub question carries 2 marks.

1.   (a) Mention the web sources available for chemical information.

      (b) How are molecular descriptors classified based on structure?

      (c) Write a short note on BLAST & FASTA.

2.   (a) Which are the steps involved in the nomenclature of drugs.

      (b) Write the mechanism of action of a water soluble drug.

      (c) What is the role of histamines?

3.   (a) What is meant by receptor binding assays?

      (b) Write a short note on Induced-fit mechanism

      (c) Explain Hill Plot.

4.   (a) Write the applications of molecular dynamics in protein folding?

      (b) List out common water and membrane models used in molecular simulation.

      (c) What is the significance of Ramachandran plot?

5.   (a) Briefly describe bond matrix.

(b) Write a note on clustering?

(c) Explain Markov process.

Section B

Answer either (a)or (b) from each question. Each question carries five marks

6. (a) Write a short note on gene therapy.

   (b) Describe a method of analysing amino acid sequence in protein.

7. (a) List and brief on different classes of drugs.

   (b) Write a short note on anti infective agents.

8. (a) Describe the action and the structure of HIV gp120.

   (b) What is the difference between Cox1 and Cox2. How is it used for rational design of Anti-inflammatory inhibitors?

9. (a) Discuss the four sequential steps in homology modeling.

   (b) Explain model building using fold recognition method.

10. (a) What are the differences between z-test,t-test and F-test?

    (b) What is the significance of correlation coefficient?

Section C

Answer any three question. Each questioncarries ten marks

11. Discuss the contribution of genomics in drug development.

12. Describe the action of Psycho pharmacological agents.

13. Write a note on GABA nergic and GPCRs?What makes it attractive as drug target.

14. Compare Langevin method, classical method and QM method.

15. Give a brief account of the statistical methods of analyzing data based on the type of data.

FOURTH SEMESTER M.Sc. DEGREE EXAMINATION

Branch : MEDICINAL CHEMISTRY

(Under Semester System w.e.f 2016 Admissions)

CM 242-ADVANCED MEDICINAL CHEMISTRY

Time: 3 hrs   Max. Marks: 75

Section A

(Answer any two among (a), (b) and (c) from each question. Each sub question carries 2 marks)

1 a) Define scaffold hopping?

   b) What is meant by pharmacophore?c) Name two softwares used for denovo drug design?

2 a) What is Single oral dose?

   b) What is prodrug?

   c) What is t-max?

3 a) Define epitopes?

b) What is rule of three?

c) What is meant by fragment self assembly?

4 a) What is SPR?

b) What are the different learning methods?

c) What is artificial neural network?

5 a) Give the structure of ketamine?

b) Write the preparation of paraldehyde?

c) Write examples of any two barbiturate drug. [2 x 10 = 20 marks]

Section B (*Answer either (a) or (b) of each question E ach question carries 5 marks)*

6 a) Explain about denovo drug design?

b) Explain about brownian dynamics?

7 a) Explain the Drug concentration analysis and its therapeutic signiûcance?

b) Explain theories of drug receptor interactions?

8 a) Explain the applications of FBDD over traditional drug design methods.

b) Account for GPCR ligands as drug targets.

9 a) Explain in detail about SOFM?

b) Explain Data Mining Techniques?

10 a) Explain the characteristic features of ideal general anaesthetics.

b) Write a note on mechanism of action and SAR of pencillin.[5x 5 = 25 marks]

Section C(*Answer any three question and each question carries 10 marks)*

11 Explain in detail about various force field models to calculate energy?

12 Explain the different quantitative models of QSAR?

13 Explain different fragment evolution methods?

14 Explain the different cheminformatic tools in HTS.

15 Write a note on the chemistry behind Drug metabolic reactions?[10x3 = 30 marks]

◆◆◆