Maharshi Dayanand University
Rohtak

Ordinances, Syllabus and Courses of Reading for

M.Sc. (Chemistry) I & II Semester

Examination

Session — 2008-2009

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M.Sc. Chemistry (Two year course)

SCHEME OF EXAMINATION w.e.f. 2008-09

M.Sc. 1st Semester

Paper No	Code No	Nomenclature	Hrs/ week	Max. Marks
I	CH-401	Inorganic Chemistry	04	80+20
II	CH-402	Physical Chemistry	04	80+20
III	CH-403	Organic Chemistry	04	80+20
IV	CH-404	General Spectroscopy	03	60+15
	Qualifying	Computer for Chemists	02	

M.Sc. 2nd Semester

Paper No	Code No	Nomenclature	Hrs/ week	Max. Marks
V	CH-405	Inorganic Chemistry	04	80+20
VI	CH-406	Physical Chemistry	04	80+20
VII	CH-407	Organic Chemistry	04	80+20
	Qualifying	Computer for Chemists	02	80+20

Practicals

VIII	CH-408	Inorganic Chemistry Practical	08	100
IX	CH-409	Physical Chemistry Practical	08	100
X	CH-410	Organic Chemistry Practical	08	100

Notes:
1. Maximum marks of M.Sc. Ist year(i.e.1st & IInd Semester will be 975 (Theory 675 marks & practicals 300 marks).
2. Computer for Chemists paper will be held at the end of 2nd Semester and will be Qualifying with pass marks 40%
3. Practical examination will be conducted at the end of IInd Semester on three consecutive days and there will be two sessions (Morning & Evening) of 04 Hrs. each Practical marks will include 10% marks for Viva-Voce and 10% for record files. The payment to the practical examiners will be made on the basis of sessions.

* Each Theory paper will include 20% marks as internal assessment as per University rules.

M.Sc. 3rd Semester

Paper No	Course No	Course	Hrs/ week	Max. Marks
XI	CH-501	Inorganic Special-I/ Physical Spl-I/ Organic Spl.-I	04	80+20
XII	CH-502	Inorganic Special-II/ Physical Spl-II/ Organic Spl.-II	04	80+20
XIII	CH-503	Inorganic Special-III/ Physical Spl-III/ Organic Spl.-III	04	80+20

M.Sc. 4th Semester

Paper No	Course No	Course	Hrs/ week	Max. Marks
XIV	CH-504	Inorganic Special-IV/ Physical Spl-IV/ Organic Spl.-IV	04	80+20
XV	CH-505	Inorganic Special-V/ Physical Spl-V/ Organic Spl.-V	04	80+20
XVI	CH-506	Inorganic Special-VI/ Physical Spl-VI/ Organic Spl.-VI	04	80+20
XVII	CH-507	Inorganic Chemistry Practicals/ Physical Chemistry Practicals/ Organic Chemistry Practicals	08	80
XVIII	CH-508	-do-	08	80
XIX	CH-509	-do-	08	140

* Each Theory paper will include 20% marks as internal assessment as per University rules.

Notes: 1. Maximum marks of M.Sc. 2nd year (i.e. IIIrd & IVth Semester will be 900 (Theory 600 marks & practicals 300 marks).

2. Practical examination will be conducted at the end of IVth Semester on three consecutive days and there will be two sessions (Morning & Evening) of 04 Hrs. each. Practical marks will include 10% marks for Viva-Voce and 10% for record files.

3. The payment to the practical examiners will be made on the basis of sessions.

M.Sc. Chemistry Ist Semester

Paper I CH-401 Inorganic Chemistry 4 hrs. / Week

Max. Marks: 80

Time: 3 Hrs.

Note:- *Examiner will set 09 questions and the candidates will be required to attempt 05 questions in all. Out of 09 questions one question will be compulsory containing 08 short answer type questions covering the entire syllabus. Further, examiner will set 02 questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks.*

Section-A

Stereochemistry and Bonding in Main Group compounds: VSEPR theory, dð -pð bonds, Bent rule and energetic of hybridization.

(7 Hrs.)

Metal-Ligand Equilibria in solution

Stepwise and overall formation constants and their interactions, trends in stepwise constants, factors affecting stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry and spectrophotometry.

(8 Hrs.)

Section-B

Reaction Mechanism of Transition Metal Complexes-I

Inert and labile complexes, Mechanisms for ligand replacement reactions, Formation of complexes from aquo ions, Ligand displacement reactions in octahedral complexes- acid hydrolysis, Base hydrolysis, racemization of tris chelate complexes, electrophilic attack on ligands.

(15 Hrs.)

Section-C

Reaction Mechanism of Transition Metal Complexes-II

Mechanism of ligand, displacement reactions in square planar complexes, the trans effect, theories of trans effect, mechanism of electron transfer reactions – types; outer sphere electron transfer mechanism and inner sphere electron transfer mechanism, electron exchange.

(15 Hrs.)

Section-D

Isopoly and Heteropoly Acids and Salts

Isopoly and Heteropoly acids and salts of Mo and W: Structures of isopoly and heteropoly anions.

(7 Hrs.)

Crystal Structures

Structures of some binary and ternary compounds such as fluorite, antifluorite, rutile, antirutile, crystobalite, layer lattices- Cd I_2, Bi I_3; Re O_3, Mn_2O_3, corundum, pervoskite, Ilmenite and Calcite.

(8 Hrs.)

M.Sc. Chemistry Ist Semester

Paper II CH-402 Physical Chemistry 4 hrs. / Week

Max. Marks: 80

Time: 3 Hrs.

Note:- *Examiner will set 09 questions and the candidates will be required to attempt 05 questions in all. Out of 09 questions one question will be compulsory containing 08 short answer type questions covering the entire syllabus. Further examiner will set 02 questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks.*

Section-A

Quantum Mechanics: Postulates of Quantum Mechanics; derivation of Schrodinger wave equation; Max-Born interpretation of yand the Heisenberg's uncertainty principle; Quantum mechanical operators and their commutations relation, Hermition operators, (elementary ideas, quantum mechanical operator for linear momentum and angular momentum as Hermition operator). The average value of the square of Hermition operators; commuting operators and uncertainty principle(x & p; E &t); Schrodinger wave equation for a particle in one dimensional box; evaluation of average position, average momentum and determination of uncertainty in position and momentum and hence Heisenberg's uncertainty principle, picorial representation of the wave equation of a particle in one dimensional box and its influence on the kinetic energy of the particle in each successive quantum level, lowest energy of the particle.

Section-B

Thermodynamics: Brief resume of first and second Law of thermodynamics. Entropy changes in reversible and irreversible processes; variation of entropy with temperature , pres-

sure and volume, entropy concept as a measure of unavailable energy and criteria for the spontaneity of reaction; free energy functions and their significance, criteria for spontaneity of a process; partial molar quantities (free energy, volume ,heat concept), Gibb's-Duhem equation;

Section-C

Chemical Dynamics: Effect of temperature on reaction rates, Rate law for opposing reactions of Ist order and IInd order, Rate law for consecutive Ist order reactions, Collision theory of reaction rates and its limitations, steric factor, Activated complex theory, Ionic reactions: single and double sphere models, influence of solvent and ionic strength, the comparison of collision and activated complex theory.

Section-D

Electrochemistry:

Ion - Ion Interactions: The Debye -Huckel theory of ion- ion interactions: potential and excess charge density as a function of distance from the central ion, Debye Huckel reciprocal length, ionic cloud and its contribution to the total potential, Debye - Huckel limiting law of activity coefficients and its limitations, ion - size effect on potential, ion -size parameter and the theoretical mean - activity coefficient in the case of ionic clouds with finite - sized ions.

Debye - Huckel -Onsager treatment for aqueous solutions and its limitations Debye-Huckel-Onsager theory for non-aqueous solutions, the solvent effect on the mobality at infinite dilution, equivalent conducftivity (Ù) vs. concentration $c^{1/2}$ as a function of the solvent, effect of ion association upon conductivity (Debye-Huckel - Bjerrum equation).

M.Sc. Chemistry Ist Semester

Paper III CH-403 Organic Chemistry 4 hrs. / Week

Max. Marks: 80+20

Time: 3 Hrs.

Note:- *Examiner will set nine questions and the candidates will be required to attempt five questions in all. Out of nine questions one question will be compulsory containing eight short answer type questions covering the entire syllabus. Further examiner will set two questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks.*

Section-A

Nature of Bonding in Organic molecules: Delocalized chemical bonding –conjugation, cross conjugation, resonance, hyperconjugation , tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule, energy level of p-molecular orbitals, annulenes, antiaromaticity, homo-aromaticity, PMO approach. Bonds weaker than covalent, addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes

Section-B

Stereochemistry : Chirality, elements of symmetry, molecules with more than one chiral centre, diastereomerism. Determination of relative and absolute configuration (octant rule excluded) with special reference to lactic acid, alanine & mandelic acid. Methods of resolution, optical purity, prochirality, enantiotopic and diastereotopic atoms, groups and faces, asymmetric synthesis, cram's rule and its modifications, prelog's rule, conformational analysis of cycloalkanes (upto six membered rings), decalins, conformations of sugars, opti-

cal activity in absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape, geometrical isomerism in alkenes and oximes, methods of determining the configuration.

Section-C

Reaction Mechanism: Structure and Reactivity: Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determing mechanisms, isotope effects. Hard and soft acids and bases. Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. Effect of structure on reactivity. The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

Section-D

Purification Techniques: Chromatography: various types of chromatography, principles and applications, counter current distribution, HPLC, electrophoresis

Natural and Synthetic Dyes: Indigo and Alizarin including their structure elucidation, interaction between dyes and fibers, various classes of synthetic dyes including heterocyclic dyes.

Dissachrides: Detailed study of maltose and lactose.

Paper IV CH -404 General Spectroscopy 90 Hrs. (3 Hrs. /week)

Max. Marks: 40

Time: 3 Hrs.

Note:-*Examiner will set 10 questions and the candidates will be required to attempt 05 questions in all. Out of 10 questions one question will be compulsory containing 08 short answer type questions covering the entire*

syllabus. Further examiner will set 03 questions from each section and the candidates will be required to attempt atleast one question from each section. All questions will carry equal marks

Section-A

1. Electromagnetic radiation, interaction of electromagnetic radiation with matter,

   regions of the

   Spectrum the width and intensity of spectral transitions. Resolving power**.**

2. **Rotational spectra**- The rotation molecules, rotational spectra of diatomic molecules, the spectrum of non-rigid rotator, the effect of isotopic substitutions, rotational spectra of linear and symmetric top polyatomic molecules

3. **Vibrational and Vibrational – Rotational Spectra**: The vibrating diatomic molecule; simple harmonic vibrations, anharmonicity of vibrations, the diatomic vibrating rotator, the interaction of rotations and vibrations, the vibrations of polyatonic molecules, analysis by infrared technique.

4. **Electronics Spectra**: Electronic spectra of idiatonic molecules, vibrational course structure, and rotational fine structure of electronic band, the Frank-Condon principle, intensity of vibrational-electronic band, dissociation energy, the Fortrat diagram.

Section-B

5. **NMR Spectra** Dynamic and magnetic properties of atomic nuclei, nuclear resonance, relaxation processeds, chemical effects in NMR e.g. chemical shift. Absorption intensities, Spin-spin coupling, Elementary idea of time dependents effects in NMR.

Instrumentation line diagram.

6. Applications of UV, IR and NMR spectra in the structural elucidation of organic compounds.

Section-C

Electronic Absorption Spectroscopy : Energy levels in diatomic molecules, introduction to electronic transition, Assignment of transitions, Spectra of transition metal complexes, Orgel diagrams, Calculation of Dq and â for Ni^{II} complexes, structural evidence from electronic spectra.
Nuclear Magnetic Resonance: Applications of spin-spin coupling to structure alignment of inorganic compounds, evaluation of reaction rates of fast exchange reactions, the double resonance technique.

Application of infra-red spectroscopy to the determination of inorganic compounds

M.Sc. Chemistry IInd Semester

Paper V CH-405 Inorganic Chemistry 4 hrs. / Week

Max. Marks: 80

Time: 3 Hrs.

Note:- *Examiner will set 09 questions and the candidates will be required to attempt 05 questions in all. Out of 09 questions one question will be compulsory containing 08 short answer type questions covering the entire syllabus. Further, examiner will set 02 questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks.*

Section-A

Metal-Ligand Bonding

Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral or square planar complexes, ð-bonding and molecular orbital theory. **(15 Hrs.)**

Section-B

Electronic Spectra of Transition Metal Complexes

Spectroscopic ground states, correlation and spin-orbit coupling in free ions for Ist series of transition metals, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1 – d^9 states) calculation of Dq, â parameters, effect of distortion on the d-orbital energy levels. Structural evidence from electronic spectrum, John-Tellar effect, Spectrochemical and nephalauxetic series, charge transfer spectra, electronic spectra of molecular addition compounds.

(16 Hrs.)

Section-C

Magnetic Properties of transition metal complexes

Elementary theory of magneto - chemistry, Guoy's method for determination of magnetic susceptibility, calculation of magnetic moments, magnetic properties of free ions, orbital contribution, effect of ligand-field, application of magneto-chemistry in structure determination, magnetic exchange coupling and spin state cross over.

(8 Hrs.)

Metal Clusters

Structure and bonding in higher boranes, Wade's rules, Carboranes, Metal Carbonyl clusters- Low Nuclearity Carbonyl clusters, total electron count (TEC)

(8 Hrs.)

Section-D

Metal -? Complexes

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structure elucida-

tion, important reactions of metal carbonyls; preparation, bonding, structure and important reactions of transition metal nitrosyl, and dinitrogen complexes; tertiary phosphine as ligand.

(15 Hrs.)

M.Sc. Chemistry IInd Semester

Paper VI CH-406 Physical Chemistry 4 hrs. / Week

Max. Marks: 80

Time: 3 Hrs.

Note:- *Examiner will set 09 questions and the candidates will be required to attempt 05 questions in all. Out of 09 questions one question will be compulsory containing 08 short answer type questions covering the entire syllabus. Further examiner will set 02 questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks.*

Section-A

Schrodinger wave equation for a particle in a three dimensional box and the concept of degeneracy of energy levels. Schrodinger wave equation for linear harmonic oscillator, solution by polynomial method, zero point energy and its consequence. Schrodinger wave equation for three dimensional Rigid rotator, energy of rigid rotator, space quantization; Schrodinger wave equaqtion for hydrogen atom, separation of variable in polar spherical coordinates and its solution. Principle, azimuthal and magnetic quantum numbers and the magnitude of their values, probability distribution function, radial distribution function and shape of atomic orbitals (s,p & d).

Section-B

Classius – Clayperon equation; law of mass action and its thermodynamic derivation. Third law of thermodynamics (Nernest heat theorem, determination of absolute entropy,

unattainability of absolute zero) and its limitation. Phase diagram for two completely miscible components systems. Eutectic systems, Calculation of eutectic point, systems forming solid compounds A_x B_y with congruent and incongruent melting points, phase diagram and thermodynamic treatment of solid solutions.

Section-C

Chain reactions: hydrogen - bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane. Photochemical reactions (hydrogen - bromine & hydrogen -chlorine reactions). General treatment of chain reactions (ortho -para hydrogen conversion and hydrogen - bromine reactions), apparent activation energy of chain reactions, chain length, Rice- Herzfeld mechanism of organic molecules, decomposition(acetaldehyde) Branching chain reactions and explosions (H_2 - O_2 reaction). Kinetics of (one intermediate) enzymatic reaction : Michaelis - Menton treatment, evaluation of Michaelis 's constant for enzyme - substrate binding by Lineweaver - Burk plot, by Dixon and by Eadie- Hofstae methods. Competitive and non-competitive inhibition.

Section-D

Ion Transport in solutions: Ionic movement under the influence of an electric field , mobility of ions, ionic drift velocity and its relation with current density, Einstein relation between the absolute mobility and diffusion coefficient, the Stokes- Einstein relation , the Nernst -Einstein equation, Waldens rule, the Rate- Process approach to ionic migration , the Rate process equation for equivalent conductivity, total driving force for ionic transport, Nernst - Planck Flux equation, ionic drift and diffusion potential , the Onsager phenomenological equations. The basic equa-

tion for the diffusion, Planck- Henderson equation for the diffusion potential.

M.Sc. Chemistry IInd Semester

Paper VII CH-407 Organic Chemistry 4 hrs. / Week

Max. Marks: 80+20

Time: 3 Hrs.

Note:- *Examiner will set 09 questions and the candidates will be required to attempt 05 questions in all. Out of 09 questions one question will be compulsory containing 08 short answer type questions covering the entire syllabus. Further examiner will set 02 questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks.*

Section-A

Aliphatic Nucleophilic Substtitution: The SN2, SN1, mixed SN1 and SN2 SNi , SN1', SN2' SNI' and SET mechanisms. The neighbouring group mechanisms, neighbouring group participation by p and s bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. Reactivity- effects of substrate structure, attacking nucleophile, leaving group and reaction medium.. Ambident nucleophile, regioselectivity. Phase transfer catalysis.

Section-B

.Aliphatic Electrophilic Substitution: Bimolecular mechanisms - SE2 and SEi. The SE1 mechanism, Electrophilic substitution accompained by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

Aromatic Electrophilic Substitution: The arenium ion mechanism, orientation and reactivity, energy profile diagrams.

The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction.

Aromatic Nucleophilic Substitution: The ArSN1, ArSN2, Benzyne and SRN1 mechanisms. Reactivity – effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

Section-C

Elimination Reactions: The E2, E1 and E1cB mechanisms . Orientation of the double bond . Reactivity –effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

Addition to Carbon-Carbon Multiple Bonds: Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio – and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring.

Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation.

Section-D

Addition to Carbon-Hetero Multiple Bonds: Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig reaction. Mechanism of condensation reactions involving enolates – Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

Paper VIII CH-408 Inorganic Chemistry Practical 240 Hrs. (8Hrs./Week)

Max. Marks: 100

Time: 8 Hrs.

1. Qualitative Analysis:
   a) Less common metal ions- Tl, Se, Te, Mo, W, Ti, Zr, U&V
   b) Insolubles- Oxides(WO_3, Silica, Alumina); Sulphates(Lead Sulphate, Barium Sulphate Strontium Sulphate and Calcium Sulphate); Halides(Calcium fluoride and silver halides)

(2 less common metal ions and 1 insoluble to be given) (30 Marks)

2. Quantitative Analysis:
   a) Separation and determination of two metal ions such as Ag- Cu, Cu- Ni, Cu- Zn, Ni- Zn, Cu-Fe etc. involving volumetric and gravimetric methods. (35 Marks)
   b) Determination of Ferrous, Oxalate, Nitrite etc. by Cerimetry (15 Marks)
3. Viva-Voce (10 Marks)
4. Note Book (10 Marks)

Paper IX CH-409 Physical Chemistry Practical 240 Hrs. (8Hrs./Week)

Max. Marks: 100

Time: 8 Hrs.

1. Conductometry

(i) Determination of cell constant

(ii) NaOH vs. HCl titration.

(iii) NaOH vs. Oxalic acid titration

(iv) NaOH vs. CH_3COOH titration.

(v) $AgNO_3$ vs. KCl titration.

(vi) $Ba(NO_3)_2$ vs. Na_2SO_4 titration.

2. Potentiometry

(i) NaOH vs. HCl titration.

(ii) NaOH vs.Oxalic acid titration.

(iii) NaOH vs. CH_3COOH titration

(iv) $AgNO_3$ vs. KCl titration.

(v) $KMnO_4$ vs. Mohr's Salt $FeSO_4$ titrations.

3. pH metry

(i) NaOH vs. HCl titration.

(ii) NaOH vs. Oxalic acid titration.

(iii) NaOH vs. CH_3COOH titration.

4. Thermochemistry

(a). Determination of heat of neutralisation

(i) NaOH vs. HCl .

(ii) NaOH vs. CH_3COOH

(iii) NaOH vs. Oxalic acid.

(b) Determination of Heat of solution and Heat of hydration of $BaCl_2$ and $CuSO_4$

5. Chemical Kinetics

(i) To study kinetics of hydrolysis of an ester in the presence of acid

(ii) To compare the relative strength of acids(HCl and H_2SO_4)

(iii) To determine the temperature coefficient for the Ist order reaction.

6 Refractometry

(i) Determination of molar refractivity of the given liquid.

(ii) To determine percentage composition of liquids in the given binary mixture.

7. **Surface Tension**

To determine interfacial tension of the two immiscible liquids.

8. **Adsorption**

i) To study the adsorption of Oxalic acid and Acetic acid on charcoal from aqueous solution.

9. **Distribution Law**

i) Determination of partition coefficient of benzoic acid between benzene and water

ii) Determination of partition coefficient of iodine between carbon tetrachloride and water

iii) Determination of equilibrium constant for $I_2 + I = I_3$

Two Experiments = 2x40	=	80 marks
Viva-Voce	=	10 marks
Note-Book	=	10 marks

Paper -X CH-410 Organic Chemistry Practical 240 Hrs. (8Hrs./Week)

Max. Marks: 100

Time: 8 Hrs.

1. Qualitative Analysis **(45 Marks)**

Separation, purification and identification of compounds of binary mixtures by chemical tests and checking purity of individual components using TLC. IR spectra to be used for functional group identification.

2. Organic synthesis

Two Step Preparations : **(35 Marks)**

p-nitroaniline from p-bromoaniline

anthranilic acid from phthalic anhydride

p-bromoacetanilide from aniline.

p-nitroacetanilide from aniline

sym-tribromoaniline from aniline

2,4-dinitrophenylhydrazine from chlorobenzene

2,5-dihydroxy acetophenone from hydroquinone

3. Viva-Voce **(10 Marks)**

4. Note Book **(10 Marks)**

Computers for Chemists **60 Hrs (2 Hrs/week)**

Max. Marks :100

Time : 2 hrs.

Essentials of Computer:

Historical Evolution of Computers, Block diagram of a Computer and functions of various units; Classification of Computers; Input/Output devices (Display Devices, Printers, etc.) Memories: RAM, ROM, Cache Memory, Virtual memory; Mass-storage Media: Magnetic Disks, Magnetic Tapes and Optical Disks; Batch processing systems, Time sharing systems, Multiprocessor, Parallel Processing Systems.

Introduction to Programming languages: 1 GL to 5 GL languages. Software and its types; Operating System with DOS as an example, Introduction to UNIX and Windows.

Overview of: Information Technology (IT), Data Communication, Computer Networks (LAN, WAN and MAN) and their applications, Introduction to Internet and Intranet technology.

Computer Applications:Scientific, Business, Research, Sports, Medicine & Health Care, Engineering, Teaching etc.

Problem Solving: Problem Identification, Analysis, flowcharts, Decision Tables, Pseudo codes and algorithms, Program Coding, Program Testing and Execution.

Computer Programming Language (FORTRAN Language) :

Elements of the computer language. Constants and variables.

Operations and symbols. Expressions. Arithmetic assignment statement. Input and Output. Format statement. Termination statements. Branching statements such as IF or GO TO statement. LOGICAL variable. Double precision variables. Subscripted variables and DIMENSION. DO statement. FUNCTION and SUBROUTINE. COMMON and DATA statements.

A brief introduction to C language.

Books Suggested

1 Computers and Common Sense, R. Hunt and J. Shelley, Prentice Hall.

2 Computational Chemistry, A.C. Norris.

3 Microcomputer Quantum Mechanics, J.P. Killngbeck,Adam Hilger.

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