VEER NARMAD SOUTH GUJARAT UNIVERSITY, SURAT.

M.Sc. Part-II

Industrial Chemistry

Paper-IV

Max. Marks: 100 (External-70 + Internal-30) To come in force from June-2004

Process Control and Instrumental Methods of Analysis

Total Period/Hours : 120

UNIT-I : **(20 hours)**

(1) UV-Visible Spectrophotometry:

Review of different electronic transition, Woodward's rules for a,B-unsaturated ketones, Diene systems, Effect of solvent on absorption bands – Elementary idea of double beam automatic recording, Spectrometer, Application of Spectroscopy to organic compound.

(2) IR Spectrophotometry:

Spectrophotometer – Components of IR Spectrophotometer – Sample handling – Calibration of wavelength – Interpretation of IR spectra using correlation charts – Study of few representative spectra, n-hexane, 2-methyl pentane, n-hexyl amine, n-butyl methyl ether, butyramide, n-hexanol, Acetophenone, n-butyl acetate, ethyl benzoate, n-hexanoic acid, benzoic acid, phenol, Effect of H-bonding on absorption bands – Elementary idea about FT-IR Spectrophotometer. Application of IR spectra and to organic compound.

UNIT-II : **(20 hours)**

(1) NMR Spectra:

Review of theory, Chemical shift, Reference and solvents used – Elementary idea about NMR spectrometer – Spin-spin coupling, Magnetic anisotropy – Chemical equivalence, Magnetic equivalence, Structure elucidation from NMR spectra – Study of NMR spectra of some illustrative compounds. Brief description of C^{13} NMR – Shift reagents.

(2) Thermal Methods of Chemical Analysis like TGA, DTA, DSC. Ref.: Instrumental Methods of Chemical Analysis by Gurdeep Chatwal & S. K. Anand.

UNIT-III : **(20 hours)**

(1) **Mass Spectrometry:**

Principle of mass spectra – Parent peak – Net stable ions – Base peak – Isotope effect of arrive at correct molecular formula – Fragmentation rules – McLafferly rearrangement – Use of mass spectra to elucidate structure of organic compounds. Mass spectra of some illustrative compounds. (Problems covering all above techniques).

2) E.S.R.S.

(a) Gas Chromatography:

UNIT - IV : (20 hours)

Selection of mobile phase – Selection of stationary phase in GLC and GSC – Detectors : FID, TCD and ECD. Their comparison, Packed, Column, WCOT, SCOT – Temperature programming – Derivatisation in GC – Quantitative Analysis.

(a) High Performance Liquid Chromatography:

Technique – Instrument and its components – Isocratic and Gradient elution – Normal phase and reversed phase HPLC – Derivatisation.

(b) Thin-Layer Chromatography:

Selection of stationary and mobile phase – Detection techniques – Elementary ide HPTLC.

UNIT-V : (20 hours)

(A) Environmental Chemistry:

Introduction, Aquatic pollution – Inorganic, Organic, Pesticide, Agricultural, Industrial and Sewage, Detergents, Oil spills, Oil Pollutants.

Water quality parameters – dissolved oxygen, biochemical oxygen demand. Analytical methods for measuring DO, BOD and COD, Heavy metals, Purification and treatment of water.

(B) Chemical and photochemical reactions in atmosphere, Smog formation, Oxides of N, C, S, 0 and their effect. Analytical methods for measuring air pollutants.

(C) Industrial pollution of sugar, Distillary, drug, Paper & pulp & polymer industries an analysis. Effluent treatment plants of above industries.

UNIT-VI : (20 hours)

Process dynamics and responses of open loop system. Closed loop systems. Development of block diagrams, Stability of control systems, Off set calculation for P, PI, PD & PID systems, Tuning of controller for open loop and closed loop systems, Linearisation of non-linear control systems, Study of advanced control system like cascade control, Ratio control, Fled forward control etc. Introduction to DCS systems, Introduction to basic concepts of computer and working with window based programmes, Application of MATCAB in process control.

REFERENCES:

(1) Application of absorption Spectroscopy of Organic Compounds, J. R. Dyer.
(2) Modern Methods of Chemical Analysis, Robert L. Pecsok & Donald Shields.
(3) Instrumental Methods of Analysis, Williard, Merit and Dean, CBS.
(4) Instrumental Methods of Chemical Analysis by Gurdeep Chatwal & Anand S. K.
(5) Environmental Chemistry by V. P. Kudesia (Pragati Prakashan, Meerut).

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M.Sc. Part-II

Industrial Chemistry
Paper-V

Max. Marks: 100 (External-70 + Internal-30) To come in force from June-2004

Dyes and Pigments

Total Period/Hours : 120

UNIT-I : Industrial Organic Pigments : (20 hours) (1)

Definition:

(A) Azo Pigments:

Monoazo pigment
Disazo pigment
(3-Napthol pigment
Napthanol AS pigment
Azo pigment lakes (Salt type pigments)
Benzimidazolone pigment
Disazo condensation pigment
Metal complex pigment
Isoindolinone & Isoindolinine pigment

(B) Polycyclic Pigments:

Phthalocyanine pigment
Quinacridone pigment
Perylene & Perinone pigment
Diketo pyrrolo, pyrrole (DPP) pigment
Thioindigo pigments

(C) Anthraquinone Pigments:

Anthra pyrimidine pigment
Flavanthrone pigment
Pyranthrone pigment
Anthranthrone pigment
Dioxazine pigments
Triaryl carbonioum pigment
Quinophthalone pigment

UNIT-II : **(20 hours)**

(a) Azo dyes – General (Diazotisation, mechanism and different methods of diazotization and laws of coupling), Monoazo, bisazo dyes, azoic dyes.

(b) Classification and methods of application of dyes. Evaluation of dyes.

UNIT-III : Anthraquinone Dyes : **(20 hours)**

Vat dyes, Acid dyes, Solubilized vat dyes, Mordant dyes and Dyes for cellulose acetate.

UNIT-IV : **(20 hours)**

(1) Non-Textile Uses of Dyes :

Leather dyes – Paper dyes – Hair dyes – Food dyes – Ink dyes – Photographic dyes – Indicator dyes – Laser dyes – Liquid crystal dyes – Solar cell, biological uses of dyes.

(2) Fluorescent Whitening Agents:

Theory of fluorescence – Classification of FWA and Synthesis of important-member of each class.

UNIT-V : **(20 hours)**

General nature, Classification, Structural variation, Synthesis and application of fibres of the following dyes:

(1) Reactive dyes
(2) TPM dyes
(3) Disperse dyes

UNIT-VI : Theories of Colour : **(20 hours)**

(a) Colour & Chemical Constitution:

Theories of colour – bathochromic and hypsochromic effect – Hyperchromic & Hypochromic effect – Witt's theory – Armstrong's theory – Nietzki's theory – Resonance theory – M.O. theory.

(b) Colour Science:

Subjective colour attributes – Hue, Lightness & Chroma (or Saturation) – Objective colour measurements – CIE Illuminant sources, CIE standard observer, Reflection spectra of object – CIE tristimulus values of colour – chromaticity diagram and co-ordinates – Correlation with visual perception of colour metamerism – CIELAB colours and colour difference tolerance limit, Shade sorting additive and substractive colour 'mixing – Kubelka-Munk theory, Introduction and useful equation only – No derivation – K-M function, K-M absorption and Scattering coefficient – Dye strength evaluation, Colour control system – Outline of construction and working of spectrophotometer – Conceptual introduction of computer colour matching (no theory).

REFERENCES:

(1) Instrumental Colour Measurement & Computer Aided Colour Matching for Textiles by H. S. Shah & R. S. Gandhi, Pub. Mahajan Book Distributors, 1990, Ahmedabad.

(2) The Chemistry of Synthetic Dyes, Vol. I to VII by Venkataraman, Academic Press, New Delhi.

(3) Chemistry of Synthetic Dyes & Pigments by Lubs.

(4) Dyes & Their Intermediates by L. N. Abrahat.

(5) Technology of Textile Processing by V. A. Shehnai, Sevak Publications, Bombay.

(6) Developments in the Chemistry and Technology of Organic Dyes by J. Griffiths, Blackwell Scientific Publication, Oxford, London.

(7) Industrial Dyes by Klans Hunger, Germany by Wiley-VCH.

(8) High-Technology Application of Organic Colorants by Peter Gregory, Plenum Press, New York.

(9) Industrial Organic Pigments by Wiley Herbst & Klans Hunger,Published by VCH, A. Wiley Company.

(10) Industrial Practice in Colour Measurements by H. S. Shah (1998), Pub. By Mahajan Publishers Pvt. Ltd., Ahmedabad.

(11) Principles of Colour Technology by Fred W. Billmeyer & Max Saltzman, John Wiley & Sons.

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M.Sc. Part-II

Industrial Chemistry

Paper-VI

Max. Marks: 100 (External-70 + Internal-30) To come in force from June-2004

Medicinal Chemistry
(Drugs)

Total Period/Hours : 120

UNIT-I : Quantitative Structure Activity Relationships (Q.S.A.R.): (20 hours)

(1) Introduction
(2) Graphs and Equations
(3) Physico-chemical Properties:
  (a) Hydrophobicity
  (b) Electronic Effects
  (c) Steric Effects
  (d) Other Physico-chemical Parameters
(4) Hansch Equation
(5) The Craig plot
(6) The Topliss scheme
(7) Bioisosteres
(8) Planning QSAR study
(9) Case study
(10) 3D QSAR:
  (a) Introduction
  (b) Defining Steric & Electrostatic fields
  (c) Relating Shape & Electronic distribution with biological activity
  (d) Hydrophobic potential
  (e) Advantages of 3D QSAR over 2D QSAR.
  (f) Potential problems of 3D QSAR.

UNIT-II : Combinatorial Synthesis : (20 hours)

(1) Introduction
(2) Combinatorial synthesis for drug optimization
(3) Combinatorial synthesis for drug discovery.
(4) Combinatorial synthesis – solid phase techniques
  (a) Solid support
  (b) The Anchor/linker.
(5) Methods of parallel synthesis
  (a) Houghton's Tea Bag procedure
  (b) Automated parallel synthesis

(6) Methods in mixed combinatorial synthesis
   (a) General principles
   (b) The mix and split method
   (c) Mix & split in the production of positional scanning libraries
(7) Isolating the active component in a Mixture — deconvolution.
(8) Structure determination of the active compounds
(9) Limitation of combinatorial synthesis
(10) Examples of combinatorial chemistry.

UNIT-III : Antibiotics : **(20 hours)**

Antibiotics that interfere with the biosynthesis of bacterial cell wall:

(1) The B-lactam antibiotics
   (a) The penicillin
   (b) The cephalosporins
(2) The non-lactam antibiotics
(3) Bacitraoin, Vancomycin and Cyoloserine

Antibiotics that interfere with the protein biosynthesis in micro-organisms:

(1) The non-lactam antibiotics
   (a) Macrolide Antibiotics : Erythromycin
   (b) Tetracyclines
   (c) Chloramphenicol
   (d) Lincomycin

Structural formulae and therapeutic uses of following non-lactam antibiotics:

(a) Aminoglycoside antibiotics
(b) Non-classifiable antibiotics. Novobiocin, Nalidixic acid, Norfloxacin, Ciprofloxacin

SAR among Penicillin and Tetracyclines.

Synthesis of Penicillin V, Ampicillin, Cephalosporin, Chloramphenicol.

UNIT-IV : **(20 hours)** (A)

Psychoactive Drugs – The Chemotherapy of mind:

CNS Depressants:

(1) General Anaesthetics
(2) Sedatives and Hypnotics
(3) Antianxiery drugs

Mode of Action of Hypnotics:

Antipsychotic drugs:

(1) Antidepressants
(2) The neurdieptics

Synthesis of only the following:

Thiophental (Pentothal), Aminobarbital (Amytal), Diazepam, Chlorazepam, Alprazolam, Glutethimide, Nikethamide.

(B) Local Anaesthetics:

Synthesis of following drugs: Cocaine, Procaine, Lidocaine (Xylocaine), Dibucaine (Nupercaine), SAR and Mode of Action of Local Anaesthetic.

(C) Analgesics:

Synthesis of following compounds: Meperidine (Pethidine), Ibuprofen, Meclofenamate sodium, Oxyphenbutazone, Paracetamol, Novalgin.

UNIV-V : Local Antiinfective Drugs: (20 hours)

(A) Antituberculosis & **Antileprotic Agents:**

Synthesis of only the following drugs:

Isoniazid (INH), Ethionamide, Ethambutol, DDS (Dasone).

(B) Sulfonamides:

Synthesis of only the following drugs:

Sulfacetamide, Sulfadiazine, Sulfadoxine (Sulfamethoxine), Sulfamethoxy-pyrazine (sulfalene), Sulfathiazole, Succinyl sulfathiazole (Sulfasuxidine), SAR and Mode of Action of Sulfonamides.

(C) **Antimalarials:** Synthesis of only

the following drugs:

Mefloquine, Chloroquine, Primaquine, Daraprim (Pyrimethamine), Quinacrine, SAR and Mode of Action of Antimalarial drugs.

UNIV-VI : (20 hours)

(A) Antineoplastic Agents (Cancer Chemotherapy:

Synthesis of only the following drugs:

Mechlorethamine, Cyclophosphamide, Melaphaian, 6-Mercaptopyrine.

(B) Antihistamine or Antiallergenic drugs:

Synthesis of only the following drugs:

Diphenyldramine (Benadryl), Antazoline, Chlorphenivamine, Pyrilamine.

(C) Diuretics:

Synthesis of only the following drugs:

Acetazolamide, Chlorothiazide, Hydroflumethiazide, Furosemide,

Ethacrynic acid. Classification and structural variation of Diuretic Drugs.

Recommended Books:

(1) Burger's Medicinal Chemistry & Drug Discovery (5/e), 1997, Vol. 1, 2, 3, 4, 5; Edited by Manfred E. Wolff (John Wiley & Sons, inc., New York).

(2) Principles of Medicinal Chemistry, Vol. I & II (5/e), by S. S. Kadam, K. R. Mahadik, K. G. Bothra (Nirali Prakashan).

(3) Principles of Medicinal Chemistry by William O. Foye (ed.), Lea & Feblyer, Philadelphia. Wilson & Glasvold's Text-book of Organic Medicinal & Pharmaceutical

(4) Chemistry (5/e, 1982) by Robert F. Doerge (S. B. Lippincott Company, Philadelphia/Toppan Co. Ltd., Tokyo).

(5) Essential of Medicinal Chemistry (2/e) by Andrejus Korolkovas (A Wiley Interscience Publication, 1988, John Wiley & Sons, Canada).

(6) Medicinal Chemistry by Ashutoshkar (Wiley Eastern Ltd., 1993).

(7) The Pharmaceutical Basis of Therapeutics by Goodman & Gilman (The Macmillan Co).

(8) The Organic Chemistry of Drugs Synthesis, Vol. I, II & III (1980), Ed. By D. Lednicer & L. A. Mitscher (John Wiley & Sons, New York).

(9) Topics in Medicinal Chemistry, Vol. I & II by Rabinowitz & Myerson (Editor) (Interscience, 1968).

(10) Adhunik Sanshleshit Aushodhonu Rasayan Vighyan, Dr. Anamik Shah, University Granth Nirman Board, Ahmedabad, Price Rs. 135/-.

(11) Introduction to Medicinal Chemistry, 2"d Edition, Graham L. Patrick — Oxford University Press.

VEER NARMAD SOUTH GUJARAT UNIVERSITY, SURAT.

M.Sc. Part-II

Industrial Chemistry

Practical
In Force From June-2005

Marks: 200 [External-120 + Internal-60 + Viva-20]

GROUP-A:

Preparation of three steps of the following organic compounds:

(i) Anthranilic acid from phthalic acid via phthalic anhydride and phthalimide.

(ii) Sulfanilamide from via p-acetamido benzene sulphonyl chloride and acetamido benzene-sulfonamide.

(iii) Eosin from phthalic acid via phthalic anhydride and fluorescein.

(iv) Benzanilide from benzene via Benzophenone and Benzophenonoxime.

(v) p-Chloro bromo benzene from acetanilide via p-bromo acetanilide and p-bromo aniline.

(vi) p-Nitro chloro benzene from acetanilide via p-nitro acetanilide and p-nitro aniline.

(vii) Benzilic acid from benzaldehyde via benzoin and benzil.

(viii) Anthrone from phthalic anhydride via o-benzoyl benzoic acid and anthraquinone.

(ix) o- and **p-hydroxy** acetophenone from aniline via phenol phenyl acetate.

(x) p-Chloro **benzoic acid** from p-nitro toluene via p-toluidine and p-chloro toluene.

(xi) **4-Methyl-7-hydroxy-8-acetyl** coumarin from resorcinol via 4-methyl-7-hydroxy coumarin and 4-methyl-7-acetyl coumarin.

(xii) Diphenyl thiourea from Nitro benzene.

(xiii) Caprolactam from cyclohexanone.

(xiv) m-Nitro phenol from Nitro benzene via m-dinitrobenzene and m-nitroaniline.

(xv) Acridone from anthranilic acid via o-chloro benzoic acid and N-phenyl **anthranilic** acid.

GROUP-B:

Use of atleast five different (a) acid dyes, (b) reactive dyes, (c) disperse dyes to dye different shades on wool, cotton and polyester fibre, yarn or fabric and to examine following parameters:

(i) dyeing at three different depth
(ii) exhaustion
(iii) fixation
(iv) light and wash fastness
(v) role of pH
(vi) role of Glauber's salt
(vii) role of temperature.

GROUP-C:

Interpretation UV-visible, IR, NMR and Mass spectra (Dry lab.).

GROUP-D:

(1) Analysis of Drugs:

(i) Sulfa-drugs by non-aqueous titration.
(ii) Novalgin.
(iii) Analysis of penicillin.
(iv) Paracetamol.

(v) Iron formulation for iron content.

(2) Determination of COD of water effluent.

(3) Determination of DO and BOD.

(4) Determination of strength of oxidizing agent like H_20_2, bleaching powder etc.

(5) Determination of strength of reducing agent sodium dithionite.

(6) Determination of temporary, permanent and total hardness of water.

(7) Determination of chemical oxygen demand of industrial effluent

(8) Analysis of organic materials: Glycerol, formalin, dye intermediate, glycine, ethylene glycol, compound.

(9) Analysis of Insecticides : Analysis of BHC.

(10) Determination of protein content of wheat flour.

(11) Analysis of bleaching material.

(12) Determination of nitrogen content of soil.

(13) Analysis of detergent sample for PO_4 and other constituents.

(14) Determination of Pb^{+2} as $PbCrO_4$ after precipitation from homogeneous solution.

(15) Electrogravimetric determination of Cu^{+2} in brass.

(16) Polarographic determination of $Cd^{+2'}$and Zn^{+2} in a mixture.

(17) Amperometric titration of (i) Pb^{+2} with $K_2Cr_2O_7$ and (ii) Ni^{+2} with DMG.

(18) Constant current coulometric determination of (i) As_2O_3 and (ii) Phenol.

(19) Biamperometric titration of iodine with $Na_2S_2O_3$.

(20) Determination of fluoride using ion selective electrode.

(21) Analysis of dye intermediate containing —NH_2 by potentiometric titration.

(22) Photometric titration of (Cu^{+2} + Ca^{+2}) in a mixture.

(23) PK In of indicator and determination of Isobestic point.

(24) Pb^{+2} with dithiozone in a water effluent

(25) Flame photometric determination of Na and K^+.

(26) Sugar in blood.

(27) TGA analysis of CaC_20_4 + MgC_2O_4

(28) Proximate analysis of coal.

(29) Quinine by fluorescence method.

(30) Biuret in a sample of urea.

(31) Silica in water.

(32) Determination of iron in dolomite and bauxite.

(33) Determination of metal:ligand ratio in complex.

(34) Analysis of ores such as Haematite, Dolomite, Lime stone, Bauxite and Pyrolusite (minimum three to be done) for their major constituents.

(35) Analysis of alloys -

(i) Cu, Zn and Fe in brass.
(ii) Cu, Ni in german silver.
(iii) Manganese in steel spectrophotometrically.
(iv) Silver alloy for silver content.

GROUP-E: Separation methods:

(i) TLC separation of amino acids.

(ii) TLC separation of dyes.

(iii) Determination of total salt content using ion-exchange resin.

(iv) To determine the ion-exchange capacity of resin.

(v) Ion-exchange separation of Fe^{+3} and Co+2

(vi) GC **separation of aliphatic hydrocarbon mixture.**

(vii) Separation of copper and nickel by electrolysis.

(viii) Extraction of Fe^{+3} and its determination.