Programme Objectives:

After studying the M.Phil. program, the students will be able to

(i) Introduce the purpose and importance of research for future development.
(ii) Know the different types of literature search and indexes.
(iii) Understand the error analysis, correlation methods and computer application
(iv) Enrich the knowledge in various types of spectral techniques and scientific analysis.
(v) Develop their skills for carrying out the project.
(vi) Make awareness in social and industrial relevant issues.
(vii) Present their findings in national and international seminars and conferences.

Programme Outcome:

After completing the M.Phil program the students will be able to

1. Pursue research program
2. Qualify as Chemist/Scientist in various industries and research Institutions
## Curriculum

### SEMESTER – I

<table>
<thead>
<tr>
<th>Course Code</th>
<th>Name of the Course</th>
<th>Hrs/week</th>
<th>Credits</th>
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<tr>
<td>19CHE701</td>
<td>Research and Teaching Methodology</td>
<td>4</td>
<td>4</td>
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<tr>
<td>19CHE702</td>
<td>Advance Scientific techniques in chemical analysis</td>
<td>5</td>
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<tr>
<td>19CHE798</td>
<td>Project oriented elective course*</td>
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<td></td>
<td>Seminar, Field work &amp; Review Writing</td>
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### SEMESTER – II

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<td>19CHE799</td>
<td>Project work, dissertation and Viva-voce</td>
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**Total Credits** 38

## LIST OF ELECTIVES

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<th>Credits</th>
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<td>Retrosynthetic Analysis</td>
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<td>19CHE732</td>
<td>Dyes and Pigments*</td>
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<td>19CHE733</td>
<td>Trends in Nanoscience and Nanotechnology*</td>
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<td>19CHE734</td>
<td>Polymer Nanocomposite*</td>
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<td>Introduction to Nanocomposites</td>
<td>3 1 0</td>
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<td>SS831</td>
<td>Polymer Science</td>
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<td>Silicon chemistry and drug design</td>
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<tr>
<td>SS819</td>
<td>Introduction to photochemistry</td>
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* Syllabus will be prepared later
Detailed Syllabus for M.Phil. in Chemistry

19CHE701  RESEARCH AND TEACHING METHODOLOGY  3 1 0 4

1. To introduce the purpose and importance of research for future development.

2. To know the various indexes and abstracts in science and technology as a source of all information in chemistry.

3. To learn the ways of carrying out literature search for current awareness and for the retrospective survey.

4. To know the methodology of writing thesis and journal articles.

5. To know about the teaching methodology for teaching the scientific concepts and techniques to students

Scientific Research Introduction to Research, Selection of a research topic, reviewing the literature, preparing the proposal and design of study Experimentation and interpretation of results. Formation, testing and rejection of hypothesis. Preparation and presentation of reports, dissertation and thesis writing.


Error Analysis Limitation of analytical methods, accuracy, precision & minimization of errors – systematic and random errors and reliability of results – Mode – Median – Mean – Standard deviation- Variance & Covariance, normal distribution and the normal probability curve Confidence interval, Q test, F test, t test, paired t test.

Correlation methods & Non-parametric tests Scatter diagram and linear regression line: Spearman rank order correlation, Pearson’s product moment correlation - Correlation coefficient. Non-parametric tests - \( \chi^2 \) test, Median test, Mann-Whitney test, Sign test, Wilcoxon on matched-pairs signed ranks test.


Reference:

2. R.O. Butlet, Preparing thesis and other manuscript.
1. To master the basic principles of spectroscopy to apply for structural elucidation.
2. To learn the methods of characterizing compounds by spectroscopic techniques.
3. To learn the various instrumental methods studying a given compound.
4. To learn the separation techniques for organic and inorganic compounds.
5. To learn about industrial analytical processes.

Absorption Spectroscopy

Applications of Advanced Organic Spectroscopy
NMR: Basic principles of two-dimensional NMR spectroscopy – HOMOCOSY, HETCOSY and NOESY spectra and their applications – use of INEPT and DEPT methods and their applications. Mass: Molecular ions, isotope peaks, fragmentation pattern – McLafferty rearrangement - measurement techniques (EI, CI, FI, FD, FAB, SIMS, MALDI) – M + 1 and M + 2 ions – calculation of molecular formula from PM+1 and PM+2 Road-map problems covering UV, IR, 1H-NMR, 13C-NMR and mass spectral data.

EPR, NQR, Raman, XPS, PES and Mossbauer Spectroscopy
Electron Paramagnetic Resonance Spectroscopy. Principles involved in EPR; Zeeman splitting, energy levels involved. Hyperfine and super-hyperfine interactions, hyperfine splitting constants, g-factor, anisotropy in $g$-value. Instrumental details. Applications of EPR spectroscopy to organic and inorganic compounds. Analysis of EPR spectra; evaluation of $g$ values and hyperfine splitting constants from EPR spectra of both organic and inorganic compounds. Spin-trap reagents like nitrones and the nature of the EPR spectra of spin-trapped compounds. EPR spectra of systems with more than one unpaired electrons, Kramer’s degeneracy, Zero field splitting. Raman spectroscopy, principled involved in Raman spectroscopy. Surface Enhanced Raman Spectroscopy (SERS) and its applications. XPS, principles and applications, PES, principles and applications. Nuclear Quadruple Resonance Spectroscopy, principles involved. Mossbauer Spectroscopy, principles involved, isomer shifts, structural elucidation.
**Diffraction & Surface Techniques:** Principles and applications of XRD, Neutron and electron diffraction – Scanning electron microscopy (SEM) - Instrumentation – applications – surface area analysis, particle size determination – Scanning Probe Microscopes – Scanning Tunneling Microscopes – Atomic force microscopes (AFM) – Principle & applications. BET and Langumir isotherm, SEM-EDX, SIMS, ISS, AES and TOF SIMS.

**Electrochemical Techniques** Polarography – Chronopotentiometry – Chronoamperometry – chronocontometry- Linear Potential Sweep voltametry – Cyclic Voltametry – Impedence Measurements – AC Voltametry – Principles and their applications, Coulometry, Pulse voltammetry, stripping techniques

**Reference:**

7. Organic Spectroscopy – William Kemp

**19CHE798 Seminar, Field work & Review Writing 4 1 0 5**

1. **Seminar** : Seminar to be delivered on a relevant theme (01 credits)
2. **Field Work** : Visit to industry/National institutes and interaction with experts.  
   (Report to be submitted) (01 credits)
3. **Review** : Preparation and submission of review article based on research papers addressing a contemporary research problem. (02 credits)
4. **Other activities** : Attending National / International workshop / Symposium / Conferences or participation for oral / poster presentation or interaction with M.Sc. students for problem solving approaches / Work of Nobel laureates in last ten years in Science. (01 credits)

**Electives**

**19CHE731 Retrosynthetic Analysis 4 0 0 4**

**Unit I Introduction**

The disconnection approach, designing a synthesis, FGI, synths, order of events, choosing a disconnection, synthesis of aromatic compounds, Chemoselectivity in synthesis – One group C-X disconnections – alcohols, ethers, sulphides, alkyl halides, Two group C-X disconnections – 1,1-, 1,2- and 1,3-difunctionalozed compounds. protection and deprotection of functional group including C-C multiple bonds
Unit II C-C bond formations and disconnections

Reversal of polarity, protecting groups in synthesis, cyclisation and radical reactions, amine synthesis, 1,1 and 1,2 C-C disconnections, synthesis of alcohols, carbonyl compounds and carboxylic acids, synthesis of other compounds from alcohols, carbonyl compounds by one group C-C disconnections, enolate chemistry.

Unit III Two group disconnections

Diels-Alder reactions, 1,3-difunctionalized and α, β-unsaturated carbonyl compounds, base catalysed reactions, 1,5-difunctionalized compounds, Michael addition and Robinson annulations, 1,2-difunctionalized compounds, methods using acyl anion equivalents, 1,4- and 1,5-difunctionalized reactions, reconnections,

Unit IV Ring synthesis

Three, four and five membered ring synthesis and retrosynthesis, pericyclic reactions for ring synthesis, radical and photochemical reactions, six membered rings, aromatic heterocycles, aromatic heterocycles with two heteroatoms, rearrangements in synthesis, electrophilic substitution reactions, named reactions in heterocyclic synthesis.

Unit V Retrosynthesis in action

Advanced strategies, retrosynthesis in industry, stereoselectivity and regioselectivity in synthesis, using alkenes, alkynes and nitro compounds in synthesis, retrosynthetic analysis and synthesis – practice problems. Seminar

Text Books:


References:


Introduction to Nanocomposites

Introduction to nanomaterial science, Interdisciplinary nature, Structure of nanomaterials, Length scales, de-Broglie wavelength & exciton Bohr radius, Fundamentals of Quantum Mechanics: wave function, Schrödinger equation, uncertainty principle, quantum wells, quantum dots, quantum wires.

Characterization techniques

Introduction to materials and characterization techniques; Spectroscopic methods-UV-Visible and vibrational spectroscopy- Infrared and Raman, Electron spectroscopies- X-ray photoelectron spectroscopy, Ultra-violet photoelectron spectroscopy, Auger electron spectroscopy; X-ray techniques- X-ray diffraction, X-ray fluorescence spectrometry; Optical microscopy, Electron microscopy- SEM, TEM; Scanning Probe microscopies- STM and AFM.
Nanocomposites

Ceramic Matrix Nanocomposites (CMNC)
Mechanical alloying, thermal spray powder method; Polymer precursor route; Spray pyrolysis; Vapour techniques (CVD and PVD) and Chemical methods, which include the sol-gel process, colloidal and precipitation approaches and the template synthesis synthesis

Metal Matrix Nanocomposites (MMNC)
Spray pyrolysis; Liquid metal infiltration; Rapid solidification; Vapour techniques (PVD, CVD); Electrodeposition and Chemical methods, which include colloidal and sol-gel processes.

Polymer Matrix Nanocomposites (PMNC)
Nanocoatings, Nano particle dispersion in polymer matrix-processing of polymer nano composites, processing of organic-inorganic hybrid materials. Intercalation of the polymer or pre-polymer from solution; In-situ intercalative polymerization; Melt intercalation; Direct mixture of polymer and particulates; Template synthesis; In-situ polymerization; Sol-gel process. Chemical and electrochemical methods.

TEXTBOOKS/ REFERENCES:
5. Z.L. Wang, Characterization of nanostructured materials
7. Nanomaterials, Nanotechnologies and Design: An Introduction for Engineers and Architects- Daniel L. Schodek, Paulo Ferreira, Michael F. Ashby ( Butterworth - Heinemann

Polymerisation mechanisms
Chemistry of condensation polymerisation, types of condensation polymers. Types of stepwise reactions. Interfacial condensation, Ring opening polymerisation reactivity and molecular size. Poly functional condensation polymerisation gelation, gel point experimental observation, Molecular weight distribution, ring scission polymerisation, Metathesis polymerisation, group transfer polymerisation
Heat and free energy of polymerisation, Cationic polymerisation – mechanisms and kinetics of anionic polymerisation, examples, kinetics and mechanism, co -ordination polymerisation, polymerisation with supported metal oxides. Different types of catalysts, kinetics of step polymerisation, copolymerisation, and reactivity ratios.

Methods of polymerisation
Copolymerization: types of copolymers, the copolymer composition equation, monomer
reactivity ratio and copolymer structure, influence of structural effectsof monomers on monomer reactivity ratios, the Q-e scheme, synthesis ofalternating, block and graft copolymers. Step reaction (condensation) polymerization-kinetics and mechanism of step reaction polymerization, Carothers equation, number distribution and weight distribution functions, polyfunctional step reaction polymerization, prediction of gel point. Controlled polymerization methods-nitroxide mediatised polymerization, AtomTransfer Radical Polymerization (ATRP), Reversible Addition Fragmentation Termination (RAFT), electrochemical polymerization, metathetical polymerization, group transfer polymerization.

**Polymer reactions**
Hydrolysis, acidolysis, aminolysis, hydrogenation, addition and substitution reactions, Reaction of various specific groups, cyclisation reaction, cross linking reactions, reactions leading to graft and block copolymer.

**Polymer viscoelasticity**, introduction to the viscoelastic properties of polymers, some simplinear viscoelastic models-Maxwell model, Voigt model, series combination of Maxwell and Voigt model, generalized linear viscoelasticity, the Boltzmann principle, the linear viscoelastic behavior of polymer solids, creep experiments, stress relaxation experiments, stress-strain experiments, oscillatory experiments, the elastic modulus, time temperature equivalence, time-temperaturesuperposition principle.

**Rheological properties of polymers** - introduction to polymer melt rheology, Newtonian fluids, non-Newtonian fluids, pseudoplastic, thixotropy, St. Venant body, dilatant, complex rheological fluids, rheopectic fluids, time dependent fluids, time independent fluids, power law, Weissenberg effect, laminar flow, turbulent flow, die swell, shark skin, viscous flow, melt flow index. Transport in polymers-diffusion, liquid and gas transport, Fick’s law, theories of diffusion.

**TEXTBOOKS/ REFERENCES:**
1. F.W. Bilmeyer, Textbook of polymer science, Wiley Interscience, 1971
4. Polymer science and technology, Fried

**Polymer processing**

**Polymerization techniques**
Bulk polymerization, solution polymerization, emulsion polymerization, suspension polymerization, interfacial polymerization, melt polycondensation, solution polycondensation, solid and gas phase polymerization.

**Polymer testing**
Importance of standards and standard organisations. Processability and performance, testing of plastics and rubbers, material characterisation tests such as melt flow index, capillary rheometer test, viscosity test, gel permeation, chromatography, and thermal analysis.
Material characterisation tests for thermosts. Apparent bulk density, bulk factor and pourability of plastics materials. Flow tests such as spiral blow, cup flow, viscosity tests for thermost resin bubble viscometer, Brookefield viscometer, gel time and peak exothermic temperature of
thermosetting resins.

**Polymer properties**
Mechanical properties: Tensile strength, flexural and compression properties, creep properties, stress relaxation, impact properties, shear strength, abrasion, fatigue and hardness etc. Thermal properties: heat deflection temperature, vicat softening temperature, torsion pendulum test, thermal conductivity, thermal expansion, brittleness temperature. Electrical properties: dielectric strength, dielectric constant, dissipation factor, electrical resistance, arc resistance etc. Weathering properties: UV, IR, X-ray, microorganisms, humidity, ozone oxygen, water, thermal energy, chemical factors. Optical properties: Refractive indices, luminous transmittance and haze, colour, gloss.

**Polymer characterisation**
Functional group analysis, use of chemical reactions and degradation for structural analysis, various microscopic techniques such as light microscopy, electron microscopy etc. and spectroscopic techniques such as IR, FTIR, NMR, EPR, UV-Visible, Raman, fluorescence etc.

**TEXTBOOKS/ REFERENCES:**
2. F.W. Bilmer, Textbook of polymer science, Wiley interscience, 1971
4. Maurice Morton, Rubber technology
5. M. Blow, Rubber Technology and Manufacture, Newness, Butterworths, 1977

**SS836 Electro and photocatalytic material 3 1 0 4**

**Unit 1: Basics of Electrochemistry**


**Unit 2: Catalysis**

Theories of catalysis: Intermediate compound formation theory of catalysis, Adsorption theory of catalysis. Heterogeneous catalysis: classic gas/solid system, the concept of the active site, promoters, modifiers and poisons. Homogeneous catalysis: elementary steps in homogeneous catalysis, ligand exchange, oxidative addition, reductive elimination, insertion and migration, de-insertion and beta –elimination, nucleophilic attack on a coordination site, industrial examples: Wacker oxidation process.

**Unit 3: Hydrogen evolution**

Advantages of electro/photo catalyst in hydrogen evolution. Difficulties in the development of electro and photocatalyst.

**Unit: 4: Materials and its characterization**

Doping with metals- nonmetals as modifiers. Dye sensitized Titania, Coupled semiconductors, conducting polymers as dopant, Supported Titania catalysts. Advanced techniques used in electrocatalysis: Electrochemical impedance analyzer-principle, OCP measurement, UV Visible spectro photometer, Photo simulator. GC analysis for hydrogen evolution rate.

**Unit5: Advanced electrochemical methods**

Principle and applications of potentio dynamic polarization. Electrochemical impedance analysis : principle, applications, Nyquist and Bode plots, Different circuit used in impedance analysis. Principle of cyclic voltametry. Linear sweep voltametry – linear potential wave form

**TEXT BOOKS/ REFERENCES:**

4. Leite, Edson Roberto; Nano Structured Materials for Electrochemical Energy
6. Antoni Llobet, “Molecular water oxidation catalysis”, Wile

**SS837**

**Industrial galvanization**

**Unit 1**

Galvanic coatings


**Unit 2**

Corrosion and its control


**Unit 3**

Corrosion Kinetics


**Unit 4**

Selection of materials for corrosive environment


**Unit 5**
Material characterization methods

TEXT BOOKS/ REFERENCES:

1. Metallurgy and Applications - David Llewellyn, Roger Hudd; Butterworth-Heinemann Publishing
2. Electrochemical methods Fundamentals and applications – Allen J. Bard, Larry R. Faulkner; John Wiley and Sons; Inc.
4. Nanotechnology Applications in coatings – Raymond H. Fernando, Li-Pin Sung; ACS
5. Introduction to materials chemistry – Harry. R. Allock: A John Wiley & sons, Inc; Publishing

SS838 Coating technology 4004

Unit 1 Introduction to Paints
General introduction to paint industry - definition of paints, varnishes and lacquers their constitution and functions, general classification of surface coatings - decorative and protective coatings,

Unit 2 Coatings
Coating methods: Roll coating, spray coating, powder coating, fluidised bed coating, electrostatic powder spray coating, electrostatic fluidised bed coating, vacuum coating, coating materials, binder oils

Unit 3 Binding media, solvents and additives

Unit 4 Adhesives
Mechanism of adhesion, mechanical interlocking, inter diffusion, adsorption and surface reaction, electrostatic attraction. Surface and interfacial properties, surface topography, surface tension and energy, wetting and setting, thermodynamic work of adhesion. Surface characterization, profilometry, low energy electron diffraction, attenuated total reflection spectroscopy, XFS, ESCA, ion scattering spectroscopy, secondary ion mass spectroscopy. Surface treatment CASING (Crosslinking by Activated Species of Inert Gas) or plasma treatment, corona discharge, acid etching, trans crystallisation growth. Interfacial chemical bonding, coupling agents, strength of adhesive joints, fracture mechanism of simple joints,
Modes of failure peeling separation, lap shear, tensile detachment from a rigid plane. Tack and auto adhesion, pressure sensitive adhesion, tackifiers, rate of peel and temperature effects in pressure sensitive adhesion, auto adhesion of elastomers.

**Unit 5 Durability and ageing**
Ageing properties of coatings, weatherometry, natural outdoor durability test accelerated outdoor weathering, artificial weathering tests, defects observed in paint film on exposure.

**TEXTBOOKS/ REFERENCES:**

**SS839 Silicon Chemistry and Drug Design 4 0 0 4**

**Unit 1 Physicochemical properties of drugs in relation to biological action**
Acid-Base Properties, Water solubility, Partition coefficient, drug administration, drug distribution, metabolism (Phase I and Phase II) and toxicity of drug receptor interaction, conformational flexibility and multiple mode of action, optical isomerism and biological activity, selected physico-chemical properties (Ionization, hydrogen bonding and biological action, chelation and biological action, oxidation - reduction potential and biological action, absorption and orientation at surfaces) Enzymes, hormones and Vitamins - representative cases, nomenclature, classification and characteristics of enzymes, mechanism of enzyme action, factors affecting enzyme action, co-factors and co-enzymes, enzymes in organic synthesis, mechanism of enzyme catalysis, enzyme inhibition.

**Unit 2 Essentials of drug design**
Molecular mimetics, drug-lead modification, drug design using QSAR and computer assisted design, assessment of drug activity, receptors and drug action, mechanism of drug action, drug metabolism pathways, Drug potentiation, drug antagonism and drug resistance

**Unit 3 Silicon in medicinal chemistry**
Organosilicon molecules with medicinal applications, chemical properties of organic silicon relevant for medicinal chemistry, silicon containing amino acids and analogues, Organosilicon based fluoride acceptors for imaging, Trialkyl silyl derivatives of drugs and biologically active molecules, Hydrophobic quaternary silanes, Increased hydrophobicity of silyl groups & effect on biological activity,

**Unit 4 Silicon derivatives**
Disilyl&disilacyclic compounds & related derivatives, spirosilanes& other silacyclic derivatives, Diphenyl silane derivatives, Silyl groups as isosteres of quaternary ammonium groups, Silyl ethers as hydrophobic substituents, silicates, silanols, silanediols&silanetriols, Hypervalent silicon compounds, stability of organo silicon compounds, silyl ethers and drug delivery strategies related to silicon, metabolism of organosilicon molecules.

**Unit 5 Medicinal agents**
Medicinal agents belonging to alkaloids, steroids, polypeptides, modified nucleic acid bases, sulphonamide and sulpha drugs, antibacterials - sulpha drugs, substituted sulphonamides, anticonvulsants, anticoagulants, antimaeobic agents, antihelmintic agents, anti-malarial agents, diuretics and cardio vascular agents, drugs for AIDS, medicinal agents affecting CNS, analgesics, antipyretics, antiseptics and disinfectants.
Unit-1 Light induced processes in everyday life

The Nature of Light, Photosynthesis, Vision, Photoresponse Mechanisms in Plants and Animals, Photomedicine, Photochemical effects of Visible and UV light, Bioluminescence, Photodegradation, Imaging processes

Unit 2 - Photochemistry - Principles and Reactions

Rates of absorption,-EinsteinBeerLaw, FluorescenceLambert’slifetimes, quantumLaw, Star yield; Fluorescence, Phosphorescence, Jablonski diagram, cis-trans isomerisation, Paterno-Buchi reaction, Norrish Type I and II reactions, photo reduction of ketones, di-pimethane rearrangement, photochemistry of arenes, Hoffmann-Loffler-Freytag reaction, Barton reaction, Photochemistry of cyclohexadienones.

Unit 3- Excited state processes

Adiabatic and Non-adiabatic processes, Monophotonic and multihotonicprocesses, Primary and secondary photochemical processes,kinetics of photochemical reactions, photo-ionization, light induced electron capture and electron transfer reactions, Intramolecular and intermolecular electron transfer, Marcus-Hush Model of Electron transfer, Electronically excited molecules-Excimers and Exciplexes, Charge transfer in excited states, twisted intramolecular charge transfer state, quenching of excited states, Stern Volmer equation, electron transfer, energy transfer, paramagnetic quenching, concentration quenching, static and dynamic quenching

Unit 4-Mechanisms of Photochemical reactions

Organic Photochemistry -Quenching, Sensitization, Unimolecular and bimolecular reactions, Photoelectrochemistry-reactions at electronically excited semiconductor electrodes, Inorganic photochemistry, photochemistry and photophysics of metal complexes, Photochemistry in solids and organized assemblies, Photochemical reactions in glasses, excitons in polymers and crystals, photochemistry in micelles, photochemical reactions of free radicals

Unit 5- Light in Industry

Photographic processes-Spectral sensitization, Colour photography, Instant photography,

TEXT BOOKS / REFERENCES:

2. Chemistry and Light- P. Suppan (RSC 1999)
3. Organic and Inorganic Photochemistry; Volume 2 of Molecular and supramolecular photochemistry - V. Ramamurthy, Kirk S. Schanze (M. Dekker, 1998)
9. Photochemistry - C. E. Wayne and R. P. Wayne (OUP Primer)