DEPARTMENT OF CHEMISTRY

ISLAMIC UNIVERSITY OF SCIENCE AND TECHNOLOGY, AWANTIPORA-192122, J&K, India

Semester-II

Overview of the Course Scheme
Second Semester

Semester	Course Code	Course Title	Course Type	Maximum Marks			Credit Distribution			Credits	Total Credits
				Internal*	Final	Total	L	T	P		
II	CHM551C	Metal Clusters and Electronic Spectra of Metal Complexes	Core	50	50	100	3	1	0	4	24
	CHM552C	Mechanism of Organic Reactions	Core	50	50	100	3	1	0	4	
	CHM553C	Quantum Chemistry, Kinetics and Statistical Thermodynamics	Core	50	50	100	3	1	0	4	
	CHM554C	Chromatographic Techniques	Core	50	50	100	3	1	0	4	
	CHM555C	Laboratory Course in Organic Chemistry	Core	50	50	100	0	0	2	2	
	CHM556C	Laboratory Course in Analytical Chemistry	Core	50	50	100	0	0	2	2	
	CHM557E	Bioinorganic Chemistry	Discipline Centric	25**	25	50	2	0	0	2	
	CHM558E	Conducting Polymers	Discipline Centric	25**	25	50	2	0	0	2	
		Choose from the list of Open Elective courses of other Departments	Open elective	25**	25	50	2	0	0	2	

*(Midterm 30 marks + Assignment 10 marks + Attendance 10 marks)
**(Midterm 15 marks + Assignment 5 marks + Attendance 5 marks)

A total of 24 credits to be taken by students with following breakup:
Core = 20 Credits
Discipline Centric =2 Credits
Open Elective =2 Credits

Second Semester
Core Course
Course Title: Metal Clusters and Electronic Spectra of Metal Complexes
Course Code: CHM551C

Credits = 4
M.M. = 100

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Unit I: Pi-Acid Complexes

Metal carbonyls, Structure and bonding, Dative overlap, Back-bonding ($p\pi$-$d\pi$) synergic interaction, Bonding and structural elucidation of metal carbonyls by IR and NMR, Important reactions of metal carbonyls, Identification of metal carbonyl isomers by IR active bands, Preparation, bonding, structure and important reactions of transition metal nitrosyl complexes. Nature and bonding of dinitrogen and dioxygen complexes.

Unit II: Metal Clusters

Occurrence and classification of metal clusters, Pre-requisites for the formation of metal-metal bond, Trinuclear compounds, Tetranuclear clusters, Polynuclear compounds , Lower halides and oxides, Metal only clusters, Bonding in metal clusters, Metal carbonyl and metal carbonyl halide clusters, Structure and bonding of compounds with metal-metal multiple bonds, Islobal analogy, Structure of some carbonyl metallocenes.

Unit III: Electronic Spectra and Magnetic Properties of Transition Metal Complexes

Spectroscopic ground states, Correlation (for d^2 system), Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1-d^9 states), Calculations of Dq, B and β parameters, Charge transfer spectra,
Types of magnetic bodies, orbital and spin effect, Curie equation and Curie Weiss law, Determination of magnetic susceptibility, Quenching of orbital Contribution, Anomalous magnetic moments, Magnetic exchange coupling and spin crossover.

Unit IV: Symmetry and Group theory

Symmetry elements and operations, Combination of symmetry operations, Groups, Subgroups, Classes, Group multiplication tables, Symmetry point groups, Identification of point groups, Systematic procedure for assignment of point groups to molecules, Symmetry classes and their geometrical significance reducible, Representations and Irreducible representations, Great orthogonally theorem (GOT), Character table (C_{2V}, $C_{3V,}$ C_{2h}).

Books Recommended:

1. Symmetry and Spectroscopy of Molecules, K. Veera Reddy, 2nd Edn.; 2009
2. Symmetry Through the Eyes of a Chemist, I. Hargittai and M. Hargittai, 3rd Edn.; 2009
3. Inorganic Chemistry; G.L. Miessler & D. A. Tarr; 3rd Edn; Pearson Edn Inc; 2004.
4. Basic organometallic Chemistry; B. D. Gupta, A J Elias; 2nd Edn; University press2013.
5. Inorganic Chemistry, J. E. Huhey, Harpes & Row. 4th Edn.; 2008.
6. Comprehensive Coordination Chemistry G. Wilkinson, R. D. Gillars and J. A. M. Clevert, 2nd Edn.; 2003.
7. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson, John Wiley 6th Edn.; 1999.
8. Symmetry and Group Theory In Chemistry, Mark Ladd, Harwood Publishers, London, Ist Edn.; 1998
9. Chemistry of the Elements, N. N. Greenwood and A. Earnshaw, Pergamon. 2nd Edn.; 1997
10. Inorganic Electronic Spectroscopy, A. B. P. Lever, Elsevier. 2nd Edn.; 1997
11. Molecular Symmetry and Group Theory, Robert L. Carter, John Wiley & Sons, 1997
12. Group Theory for Chemists, G. Davidson, Macmillan Physical Science Series, Ist Edn.; 1991.
13. Chemical Applications of Group Theory, F. A. Cotton, Wiley NY, 3rd Edn.; 1990
14. Magnetochemsitry, R. L. Carlin, Springer Verlag, 1986

Second Semester
Core Course
Course Title: Mechanism of Organic Reactions
Course Code: CHM552C

Credits = 4
M.M = 100

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Unit I: Substitution Reactions:

Review and recapitulation: Aliphatic nucleophillic: S_N1, S_N2, Walden inversion, Mixed S_N1, S_N2, S_NI and SET mechanisms, Effect of leaving group and solvent. Substitution at allylic, benzylic and vinylic carbon atoms.
Aromatic electrophillic: The Arenium ion mechanism, Energy profile diagrams, ortho/para and meta-directing groups. Ipso attack, Vilsmeir, Gatterman-Koch, Reimer-Tiemann reactions, Diazonium coupling.
Aromatic nucleophillic: Introduction to different mechanisms of aromatic nucleophilic substitution, S_NAr. Benzyne mechanism.

Unit II: Elimination Reactions

Competition between substitution and elimination reactions. The E_1, E_2 and E_1CB mechanisms and orientation of the double bond. Saytzeff and Hoffman's rule. Effect of substrate structure, attacking base, leaving group and medium. Stereochemistry of elimination reactions, elimination in cyclic systems.
Mechanistic insights of some elimination reactions: Hydro-alkoxy-elimination, *epi*-oxy-elimination, Chugaev elimination, Hoffman elimination, Cope's elimination, Shapiro reaction, Bamford-Stevens reaction, Corey-winter reaction.

Unit III: Addition Reactions

Addition to carbon-carbon multiple bond: Addition reaction involving electrophiles, Markownikov's and anti-Markownikov's rule (Peroxide effect), Nucleophiles and free radicals, Addition to cyclopropanes, Hydrogenation of double bond and triple bonds. Hydrogenation of aromatic rings, Hydroboration, Michael addition.
Addition to carbon-hetero multiple bonds: Overview of reactive carbonyl compounds, Mechanisms of addition of H_2O, HCN, Alcohols, Amines, Addition of Hydrazine, Hydrides to aldehydes and ketones. Mechanism of Wittig, Mannich, Aldol, Cross Aldol, Cannizarro, Knoevenagel, Robinson annulation, Claisen, Benzoin and Perkin reactions.

Unit IV: Molecular Rearrangement Reactions

Classification and general mechanistic treatment of electrophilic, nucleophilic and free radical moleculer rearrangement. Molecular rearrangements in acyclic, monocyclic and bicyclic carbocations. Mechanism of the following rearrangement: Wagner-Meerwin, Pinacol-Pinacolone, Demyanov ring contraction and ring expansion, Benzil-benzillic acid, Favorski, Hoffman, Curtius, Lossen, Schmidt, Beckmann, Baeyer-Villiger.

Books Recommended:

1. Fundamentals of Organic Chemjstry; Solomons; Wiley; 12th Edn.; 2015.
2. Organic Chemistry, John McMurry; Brooks/Cole; 9th Edn.; 2015
3. Advanced Organic Chemistry, Reactions, Mechanism and Structure, Jerry March, 7th Edn.; 2013.
4. Organic Chemistry, Paula Yurkanis Bruce, Pearson; 7 Edn.; 2012.
5. Advanced Organic Chemistry; 5th edn.; F. A. Carey and R. J. Sundberg; Springer Plenum; 2007.
6. Organic Chemistry; J. Hornback; Brooks/Cole; 2nd Edn.; 2005.
7. Structure and Mechanism in Organic Chemistry; C. K. Ingold; CBS; 2nd Edn.; 2000.
8. Reaction Mechanism in Organic Chemistry; S. M. Mukherjee and S. P. Singh; Macmillan; 3rd Edn.; 1998.
9. A Guide Book to Mechanism in Organic Chemistry; Peter Sykes; Longman; 6th Edn.; 1996.
10. Organic Chemistry, J. Clayden, N. Greeves and S. Warren. Oxford University Press, 2nd Edn.; 2016.

Second Semester
Core Course
Course Title: Quantum Chemistry, Kinetics and Statistical Thermodynamics
Course Code: CHM553C

Credits = 4
M.M. = 100

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Unit I: Quantum Chemistry-III

Variation theorem, Linear variation principle, Application to Hydrogen atom and Helium atom, Perturbation theory-first order (non-degenerate and degenerate), Application of perturbation method to Helium atom, Chemical bonding, LCAO-MO approximation, H_2^+ molecular ion, Brief introduction to H_2, Molecular term symbols, Valence bond treatment of H_2, Comparison of MO and VB methods in the light of H_2 molecule, Hybridization of orbitals (sp, sp^2 and sp^3).

Unit III: Chemical Kinetics-I

Kinetic analysis of experimental dat**a:** Estimation of order and rate constant from concentration-time data (Differential rate method and Integral rate method).
Fast reactions: General features of fast reactions, Study of fast reactions by flow method, Relaxation method and flash photolysis.
Theories of chemical reactions: Activated complex theory of reaction rates, Statistical and thermodynamic formulations, Comparison with collision theory.
Theories of unimolecular reactions (Lindman, Hinshelwood theories), Potential energy surfaces.

Unit IV: Chemical Kinetics–II

Surface Reactions: Unimolecular& bimolecular surface reactions, Langmuir-Hinshelwood and Langnuir-Riedel mechanism, Classical and Statistical treatments.
Reactions in liquid solutions: Diffusion controlled reactions (partial and full microscopic diffusion control), Ionic reactions: Single and double sphere models of ionic reactions, Hammett equation, Catalysis: introduction to catalysis, Mechanism of catalysis, Use of solvents as catalysts, Enzyme catalysis, Michaelis–Menten Equation, Inhibition , Effects of pH and Temperature on enzyme catalysis reactions.

Unit IV: Statistical Thermodynamics-I

Concept of Distribution, thermodynamic probability and most probable distribution, Sterling approximation, Derivation of Boltzmann distribution law, Bose-Einstein and Fermi-Dirac distribution equations (without derivation). Comparison of M-B, F-D and B-E distribution laws, Partition function and its significance, translational, rotational, vibrational and electronic partition function, Calculation of thermodynamic properties in terms of partition functions, application to ideal monoatomic gas, Equilibrium constant in terms of Partition Functions, Application to dissociation equilibrium.

Books Recommended:

1. Quantum Chemistry, D. A. McQuarie, Viva Books Pvt Ltd,Student Edn.; 2018.
2. Quantum Chemistry- Ira. N. Levine, Prentice Hall, 7th Edn.; 2013.
3. Quantum Chemistry, Prasad, New Age Publishers, 4th Edn.; 2010 (Reprint 2014).
4. Molecular Quantum Mechanics- P. W. Atkins and R. S. Friedmann, Oxford, 5th Edn.; 2010.
5. Chemical Kinetics, K. J. Laidler, Mcgraw-Hill, 4th Edn.; Revised, 2002
6. Chemical Kinetics and Catalysis, R. I. Masel, Wiley, 2001.
7. Chemical Kinetics and Dynamics, J. I. Steinfeld, J. S. Francisco, W. L. Hase, 2nd Edn.; 1998.
8. Statisdtical Thermodynamics, M. C. Gupta, New Age Publishers Pvt Ltd., 2013
9. Statistical Thermodynamics by T. L.Hill, Dover publications, 2012.
10. Statistical Mechanic by D. A. McQuarie, Viva Books Pvt Ltd, 2018.
11. Physical Chemistry, P. W. Atkins, J. D, Paula, Oxford, 2010

Second Semester
Core Course
Course Title: Chromatographic Techniques
Course Code: CHM554C

Credits = 4
M.M. = 100

Unit I: Thin-Layer Chromatography

General introduction to chromatography, Principle of TLC; Types and selection of stationary phases (adsorbents) and mobile phases, Methods of plate development; Detection of spots; Performance characteristics of thin-layer plates, Retardation and retention factor, Plate heights, 2D TLC and HPTLC, Application
Chiral chromatography: Chiral derivatization, Chiral mobile-phase, Chiral stationary phases, Mechanism of chiral interactions, Applications.

Unit II: Size Exclusion and Ion Exchange Chromatography

Principle; Gels, Theoretical basis, Exclusion limit, Total permeation and selective permeation regions. Relation between elution volume and molecular weight, Molecular weight determination. Fractionation in a complex mixture, Packing materials and applications,
Introduction to ion-exchange chromatography, Types of ion exchange materials, Mechanism of ion exchange, Ion exchange equilibrium, Total, Apparent and volume ion exchange capacity, Ion chromatography. Distinction between ion-exchange and ion chromatography, Ion suppressor Column, Applications of IEC for separation of biological molecules (amino acids).

Unit III: High Performance Liquid Chromatography (HPLC)

Principle, Theory and instrumentation, Plate theory, Rate theory, Van-Deemter-Equation, Resolution, Retention time and other basic parameters, Basic difference between HPLC and conventional liquid-chromatography, Packing materials and equipment, Detectors (UV-Vis, RI, Florescence, electrochemical) , Advantages and Applications, Reverse phase HPLC and normal phase HPLC, Brief Introduction to hyphenated LC-MS technique.

Unit IV: Gas Chromatography

Principle, Instrumentation: Columns and stationary phases, Detectors:- TCD, FID and Electron Capture Detector, Factors affecting the efficiency of the column, Van-Deemter Equation, Qualitative and qantitative analysis based on peak height and peak area, Brief introduction to hyphenated GC-MS technique.

Books Recommended:

1. Analytical Chemistry by G. D. Christian, John Wiley & Sons Inc, Singapore., 7th Edn.; 2013.
2. Gas Chromatography and Mass Spectrometry: A Practical Guide, O David Sparkman, Zelda Penton and Fulton G. Kitson, Elsevier, 2nd Edn.; 2011.
3. Introduction to Modern Liquid Chromatography: L. R. Snyder& J. J. Kirkland (John Wiley & Sons, New York). 3rd Edn.; 2009
4. Chromatography: Concepts and Contrasts, James M. Miller, Wiley, 2nd Edn.; 2009.
5. Principles of Instrumental Analysis, Skoog, Holler, Nieman, 6th Edn.; 2006
6. Principles and Practice of Analytical Chemistry by F. W. Fifield and D. Kealey, Blackwell Science Ltd, New Delhi 5th Edn.; 2004.
7. Handbook of Instrumental Techniques for Analytical Chemistry, Editor, F. Settle, Pearson Education Inc, New Delhi. Low Price Edn, 2004.
8. Instrumental Methods of Analysis, Willard, Merit, Dean and Settle, CBS Publishers and Distributors, 7th Edn.; 2004.
9. Chiral Separations by liquid chromatography and related technologies, Hassan Y. Aboul-Enein, Imran Ali, CRC press, 2003.
10. Chromatography and Separation Science By Satinder Ahuja McGraw Hill Pub, 5th Edn.; 1985.
11. Chromatographic Methods by A.Braithwaite and F.J.Smith by Kluwer Academic Publishers 5th Edn,;1999

Second Semester
Core course
Course Title: Laboratory Course in Organic Chemistry
Course Code: CHM555C

Credits = 2
M.M. = 100

Organic Preparations

1. Preparation of dibenzal acetone from benzaldehyde.
2. Preparation of adipic acid by chromic acid oxidation of cyclohexanol.
3. Preparation of caprolactum.
4. Preparation of phenol formaldehyde resin.
5. Preparation of cinnamic acid by perkin reaction.

Qualitative Analysis.

6. Detection of elements: nitrogen, sulphur and halogens.
7. Detection of functional groups: detection of carbohydrates, Unsaturation, Carboxylic acids, Carbonyl compounds, Phenols, Alcohols, Halides, Amines, Amides, Imides, Ureas, Thioureas, Nitrocompounds and hydrocarbons.
8. Separation and identification of binary organic compounds using physico-chemical methods.

Books Recommended:

1. Organic Chemistry Lab Manual N. S. Gnanapragasam and B. Ramamoorthy, S. Visvanathan Printers & Publishers, 2010.
2. Comprehensive Practical Organic Chemistry; V. K. Ahluwalia and Renu Aggarwal; University Press; 2000
3. Advanced Practical Organic Chemistry; N. K. Vishnoi; Vikas; 2nd Edn.; 1999.
4. Vogel's Textbook of Practical Organic Chemistry; A. R. Tatchell; ELBS; 5th Edn.; 1996.
5. Experiments and Techniques in Organic Chemistry; D. Pasto, C. Johnson and M. Miller; Prentice-hall; 1992.
6. Microscale and Macroscale Organic Experiments; K. L. Williamson; D. C. Heath and Co. 1989.

Second Semester
Core Course
Course Title: Laboratory Course in Analytical Chemistry
Course Code: CHM556C

Credits = 2
M.M. = 100

pH-metry

1. Determination of strength and pKa value of a weak acid by titration with an alkali.
2. Titration of a dibasic acid with alkali to find its pKa values.

Ion Exchange

3. Determination of Ion-exchange capacity of resin (cationic and anionic).
4. Separation of Zn and Cd by ion-exchangers.

Chromatography

5. Column chromatographic separation of cis and trans azobenzene and o- and p- nitoanilines determined spectrophotometrically
6. Separation of amino acids by thin layer and paper chromatography.

Spectroscopy

7. Extraction of caffeine from tea leaves, characterization by IR.
8. Determination of iron in pharmaceutical samples by visible spectrophotometry.

Quantitative analysis

9. Determination of iodine value and saponification value of edible oils.
10. Determination of metal ions by flame photometry (sodium, potassium, sodium and potassium in a mixture).

Synthesis

11. To synthesis polymer based hydrogel and determine its hydration.
12. To synthesize ion exchange material and determine the ion exchange capacity for Na^+ ions

Books Recommended:

1. Environmental Chemistry, A. K. De, 7th Edn.; 2010.
2. Fundamental of Analytical Chemistry, Skoog and Wesst, 9th Edn, 2014.
3. Practical Pharmaceutical Chemistry, part-2, Beckette, Stenlake, 4th Edn.; 2001.
4. Analytical Chemistry Thoery and Practice, R. M. Verma .CBS Publishers & Distrbutors, 3rd Edn.; 2000.
5. Vogel's Quantitative Analysis Mendham, Denny; Pearson Education 6th Edn.; 2000
6. A textbook of Practical Organic Chemistry, A. I. Vogel, 5th Edn.; 1996.
7. Standard methods of Chemical Analysis, F. J. Welcher, 6th Edn.; 1962.
8. Experiments in Chemistry, D. V. Jagirdar, Himalaya publication.

Second Semester
Discipline Centric Course
Course Title: Bioinorganic Chemistry
Course Code: CHM557E

Credits =2
M.M. = 50

Unit I: Metal ions in Biochemical Systems

Introduction to bio-inorganic chemistry, Concept of essentiality, Criteria and classification of essential elements as per their role in living systems, Bulk metals and trace metals, Role of alkali and alkaline earth metals in biosystems, Metal ion toxicity, Na^+-K^+ pump, Transport and storage of Iron (Ferritin, Transferrin and siderophores), Application of radioactive elements for biosystems.

Unit II: Metalloporphyrins and Respiration

Metalloporphyrins, Cytochromes (Cytochromes C, Cytochrome C-oxidase, Cytochrome P-450). Dioxygen transport (haemocyanin and hemoerythrin), Structure and physiological role of hemoglobin and myoglobin, Bohr Effect and cooperativity, Chloride effect.

Unit III: Electron Transport in Biosystems

Electron transport in biosystems, Iron-Sulfur proteins, Ferredoxins, Rubredoxin, Copper proteins, Photosynthesis (PS I and PS II), Z-scheme, Structure of chlorophyll a and b, Superoxide dismutase-A

Unit IV: Enzymes and medicinal Chemistry

Enzymes and co-enzymes, Structure and function of carboxypeptidase A, Carbonic anhydrase, Xanthine oxidase, Vitamin B-12, Nitrogen fixation, Biochemical basis of essential metal deficient diseases and their therapies (Iron, Zinc, Copper and Manganese). Chelate therapy, Anticancer drugs-cisplatin.

Books Recommended:

1. Inorganic Chemistry – Puri, Sharma and Kalia. Milestone publishers, 32nd Edn.; 2014
2. Inorganic Chemistry, J. E. Huhey, Harpes & Row. 4th Edn.; 2008.
3. Bio inorganic Chemistry ; K. Hussain Reddy; New Age International (P) Ltd; 2005.
4. Metal -Ions in Biochemistry; P. K. Bhattacharya; Narosa Publishing House; 2005.
5. Inorganic Chemistry in Biology; Wilkins C & Wilkins G; Oxford; 1997.
6. Principles of Bio inorganic Chemistry; Lippard, Berg; Univ. Science Books; 1994.
7. The Biological Chemistry of Elements; Frausto de Silva; Williams; Clarenden; 1991
8. A Text book of Medicinal aspects of Bioinorganic Chemistry; Das; CBS; 1990.
9. Bio inorganic Chemistry -An introduction; Ochai, Allyn and Bacon; 1977.
10. Inorganic Aspects of Biological and Organic Chemistry; Hanzilik; Academic; 1976
11. Inorganic Bio-chemistry—Vol. 1&2; Eichhorn; Elsevier, 1973.
12. The Inorganic Chemistry of Biological processes; Hughes ; Wiley; 2nd Edn.; 1973.

Second Semester
Discipline Centric Course
Course Title: Conducting Polymers
Course Code: CHM558E

Credits = 2
M.M. = 50

Unit I: Basic Concepts

Basics of conducting polymers, Historical background. Classification of electrochemically active polymers, Redox polymers, Electronically conducting polymers (Intrinsically Conducting Polymers—ICPs), Electronically conducting polymers with built-in or pendant redox functionalities, Copolymers, Composite materials, Applications of conducting polymers.

Unit II: Synthesis

Electrolytic conduction, Electrodes and mechanism; Electrochemical-synthesis of derivatives of poly-pyrrole, Polythiophene, Polyazulene, Polycarbazole, inser inorganic examples.

Unit III: Semiconducting and Metallic Polymers

Introduction and structural basis for semiconducting, metallic polymers and organic meta-polymers- synthetic routes, isomers and electronic structure of polyacetylene, Poly-*p*-phenylene, Polypyrrole, Polythiophene, inser metallic examples

Unit IV: Doping and Catalysis

Introduction, Electrochemical doping, Role of reduction and oxidation potential in doping, Polyacetylene as electrode materials.
Introduction to catalysis, Catalytic properties of conducting polymers, Catalysis of electron donor-acceptor complexes. Electrocatalysis by semiconducting polymers.

Books Recommended:

1. Conducting Polymers; A New Era in Electrochemistry, Gyorgy Inzelt, Springer-Verlag Berlin Heidelberg 2nd Edn.; 2012.
2. Conductive Electroactive Polymers, Wallace Gordon, Gordon G Wallace, Geoffrey M Spinks, CRC Press, 3rd Edn..; 2008
3. Conductive Polymers and Plastics, Larry Rupprecht, Elsevier, Ist Edn.; 2000.
4. Handbook of Conducting Polymers, Terje A. Skotheim, Ronald L. Elsenbaumer, John R. Reynolds, Marcel Dekkar, 2nd Edn.; 1997.
5. Handbook of Organic Conductive Molecules and Polymers, Four Volume Set, Hari Singh Nalwa (Editor), Wiley, 1997.
6. Organic Conductors, Jean-Pierre Farges, Marcel Dekkar, 1994
7. New Concepts in Polymer Science, Polymeric Composites, Raymond B Seymour, VSP, 1990.
8. Electrically Conductive Organic Polymers for Advanced Applications David B Cotts, Z Reyes, 1987.