Chemical bond and crystal field theory

Science, Physics



TextBooks Sr No T-1 T-2 Title Engineering Chemistry Chemistry Reference Books Sr No R-1 Other Reading Sr No OR-1 OR-2 OR-3 OR-4 OR-5 OR-6 OR-7 Journals articles as Compulsary reading (specific articles, complete reference) http://onlinelibrary. wiley. com/journal/10. 1002/(ISSN)1097-4601, http://www.springer.com/chemistry/electrochemistry/journal/10800, http://www.sciencedirect.com/science/journal/13882481, http://www. springerlink. com/content/100224/, http://www.sciencedirect. com/science/journal/00108545, http://pubs.acs.org/journal/joceah, http://www.sciencedirect.com/science/journal/00323861, Title Author Edition 1st Year 2011 Publisher Name Cengage Learning Chemistry-Concepts and Applications Steven S. Zumdahl Author Suba Ramesh, S. Vairam, P. Kalyani Raymond Chang Edition 1st 9th Year 2011 2008 Publisher Name Wiley Tata McGraw Hill Relevant Websites Sr No RW-1 RW-2 RW-3 RW-4 RW-5 RW-6 (Web address) (only if relevant to the course) http://www. klte. hu/~lenteg/animate. html http://dwb4. unl. edu/chemAnime/atomic orbits. htm http://www. mhhe.

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mit. edu/courses/chemistry/5-111-principles-of-chemical-science-fall2008/ video-lectures/lecture-28/ http://www.chem. uwimona. edu. jm: 1104/courses/CFT. html http://ocw. mit. edu/courses/chemistry/5-111principles-of-chemical-science-fall2008/video-lectures/lecture-30/ Classification of acid -base Autoionization of Water, pH Function, Strength of Acids and Bases, Equilibrium Involving Weak Acids and bases pH of salt solutions, buffers, Common ion effect, Acid-base titration. Introduction of coordination compounds, Nomenclature, Crystal Field Theory in octahedral complexes CFT Application of crystal field theory in magnetic properties and colour of the complex LTP week distribution: (LTP Weeks) Weeks before MTE Weeks After MTE Spill Over 7 6 2 Detailed Plan For Lectures Week Number Lecture Number Broad Topic(Sub Topic) Chapters/Sections of Text/reference books Other Readings, Lecture Description Relevant Websites, Audio Visual Aids, software and Virtual Labs Introduction to syllabus and general discussion on chemical principles Discovery of electron and nucleus Introduction to syllabus and general discussion on chemical principles Discovery of electron and nucleus Learning Outcomes Pedagogical Tool Demonstration/ Case Study / Images / animation / ppt etc. Planned AV17 Week 1 Lecture 1 Atoms and Molecules (Importance T-1: Ch 1 Page 14-15 of chemical principles, Discovery and 25 section 1. 6 of electron and nucleus, Waveand 1. 9 particle duality of light and matter) R-1: Ch 1 Page 25-27 Section 1. 5 Atoms and Molecules (Importance T-1: Ch 1 Page 14-15 of chemical principles, Discovery and 25 section 1. 6 of electron and nucleus, Waveand 1. 9 particle duality of light and matter) R-1: Ch 1 Page 25-27 Section 1. 5 Making them aware about the syllabus and its importance

Lecture 2 Making them aware about the syllabus and its importance AV17 Week 1 Lecture 2 Atoms and Molecules (Schrodinger T-1: Ch 1 Page 14-15 equation, Quantum and 25 section 1. 6 numbers, Concept of wavefunction 1. 9 and Ch 1 Page 32 and orbitals) -35 Section 1. 11 T-2: Ch 7 Page 279283 Section 7. 4and Ch 7 Page 286-287 Section 7. 6 Atoms and Molecules (Schrodinger T-1: Ch 1 Page 14-15 equation, Quantum and 25 section 1. 6 numbers, Concept of wavefunction 1. 9 and Ch 1 Page 32 and orbitals) -35 Section 1. 11 T-2: Ch 7 Page 279283 Section 7. 4and Ch 7 Page 286-287 Section 7. 6 Atoms and Molecules (Schrodinger T-1: Ch 1 Page 14-15 equation, Quantum and 25 section 1. 6 numbers, Concept of wavefunction 1. 9 and Ch 1 Page 32 and orbitals) -35 Section 1. 11 T-2: Ch 7 Page 279283 Section 7. 4and Ch 7 Page 286-287 Section 7. 6 Atoms and Molecules (Mulitelectron atoms and electron configurations) T-1: Ch 1 Page 27-31 35-40 Section 1. 10 1. 12-1. 13 De Broglie Equation, Limitation and numerical Schrodinger equation only and its Importance To explain particle and AV18 wave nature of matter and concept of wavefunctions, orbitals Lecture 3 De Broglie Equation, Limitation and numerical Schrodinger equation only and its Importance To explain particle and AV18 wave nature of matter and concept of wavefunctions, orbitals Week 2 Lecture 4 De Broglie Equation, Limitation and numerical Schrodinger equation only and its Importance To explain particle and AV18 wave nature of matter and concept of wavefunctions, orbitals spd orbitals shapes orientations including s p and d orbitals shapes orientations including nodes Electronic configuration of elements up to 30 atomic number using three building up principles Aufbaus rule Pauli Exclusion principle Hunds rule of maximum multiplicity Only

electronegativity Pauling Concepts of Electronegativity To introduce the AV19 20 21 concept of orbital to define the arrangement of electrons at different energy level within an atom Lecture 5 Atoms and Molecules (Electronegativity concepts, periodic properties) T-1: Ch A Page 87-91 Section A. 1 A. 2 T-2: Ch 7 Page 358375 To provide how does a AV24 covalent bond develop HW1 allotment ionic character Week 2 Lecture 5 Chemical Bonding(Covalent bonds, ionic bonds (Fajan's rule)) T-1: Ch A Page 87-88 Section A. 1 A. 2 and Ch 2 Page 49-54 Section 2. 1-2. 2 T-2: Ch 9 Page 366369 Section 9. 4 T-1: Ch A Page 87-88 Section A. 1 A. 2 and Ch 2 Page 49-54 Section 2. 1-2. 2 T-2: Ch 9 Page 366369 Section 9. 4 T-1: Ch A Page 87-91 Section A. 1 A. 2 T-2: Ch 7 Page 358375 T-1: Ch 2 Page 58-64 T-2: Ch 10 Page 417429 T-1: Ch 2 Page 64-67 Section 2. 6 T-2: Ch 10 Page 429 -432 Section 10. 6 T-1: Ch 2 Page 67-70 Section 2. 6 T-2: Ch 10 Page 432437 Section 10. 7 RW-3 Lewis dot symbols Ionic bond Polar Non polar Covalent bonds and Comparision of the properties of covalent and ionic compounds, Fajans Rule Lewis dot symbols Ionic bond Polar Non polar Covalent bonds and Comparision of the properties of covalent and ionic compounds, Fajans Rule Only electronegativity Pauling Concepts of Electronegativity To provide what type of AV22 23 bonding exist between various atoms to form a molecule Lecture 6 Chemical Bonding(Covalent bonds, ionic bonds (Fajan's rule)) To provide what type of AV22 23 bonding exist between various atoms to form a molecule Atoms and Molecules (Electronegativity concepts, periodic properties) To provide how does a AV24 covalent bond develop HW1 allotment ionic character Week 3 Lecture 7 Chemical Bonding(hybridization and shapes of molecules) sp sp2 and sp3 hybridization and their examples

Concept BMO ABMO Bond Order Magnetic character To determine how do AV25 various atoms combine to form a molecule To define the existence AV26 stability and property magnetic character of molecule To define the existence AV27 stability and property magnetic character of molecule Lecture 8 Chemical Bonding(Molecular orbital theory) RW-4 Lecture 9 Chemical Bonding(molecular orbital diagram for homonuclear diatomic molecules) MO diagram Bond order and magnetic character of Homonuclear diatomic molecule only Week 4 Lecture 10 Solid state(Idea of spatial T-1: Ch 3 Page 95-97 periodicity of lattices, band theory) Section 3. 1-3. 2 Amorphous and To define the nature of crystalline substance unit the substance formed cell Space Lattice due to arrangement of atoms or molecules Band theory Conduction To explain the electrical valence band Energy property of different Gap Application in substances Conductors Band theory Conduction To explain the electrical HW 1 submission valence band Energy property of different Gap Application in substances Semiconductor Types n and p, Insulators Lecture 11 Solid state(Electrical properties of material like conductor) T-1: Ch B Page 142144 Section B. 3-B. 4 T-2: Ch 20 Page 876878 Section 20. 3 T-1: Ch B Page 145 Section B. 4 T-2: Ch 20 Page 876878 Section 20. 3 Lecture 12 Solid state(semiconductor and insulator) Week 5 Lecture 13 Chemical dynamics and Catalysis (Rate laws, nuclear chemistry and elementary reactions) T-1: Ch 6 Page 261268 Section 6. 1-6. 3 T-2: Ch 13 Page 546 — 564 567 Section 13. 1-13. 3 T-1: Ch 6 Page 287289 Section 6. 6 T-2: Ch 13 Page 568571 Section 13. 4 RW-5 Rate Order of reactions Units of Rate constant Rate law Integrated rate Law derivation amp numerical based on zero amp first Order reactions To have the

understanding of reaction the stochiometry of reactants to form products AV28 Lecture 14 Chemical dynamics and Catalysis (Collision theory, Arrhenius concept, application of transition state theory (Energy profile diagram)) Collision theory and To explain how do factors affecting it, No various reactions takes Derivation Arhenius place equation terms Activation energy Energy profile diagrams including intermediate and transition state reaction mechanism and To explain the sequence AV29 its evidence of steps in a reaction and verification of proposed mechanism Lecture 15 Chemical dynamics and Catalysis (Reaction mechanism) T-1: Ch 6 Page 281286 289 Section 6. 56. 6 T-2: Ch 13 Page 571581 Section 13. 4 and 13. 5 T-1: Ch 13 Page 581 and 586-588. Section 13. 6 T-2: Ch 14 Page 737738 Week 6 Lecture 16 Chemical dynamics and Catalysis (Enzyme catalysis) enzyme catalysis, Protein To explain the increase AV30 chain peptidase in rate of reaction due Test 1 Allotment to substance without being consumed itself during the course of reaction taking enzyme catalysis Homework, Test 1 RW-6 Reduction amp oxidation To provide basics of Oxidizing and reducing electrochemistry To agents Oxidation number provide basics of electron transfer Balancing redox reaction reactions by ion electron method Galvanic cell Anode cathode Salt bridge and its significance Standard reduction potential and SHE Application of series Analytical numerical To explain how a chemical reaction is used to generate electricity and to provide possible combination of reactants in order to generate electricity AV31 32 Lecture 17 Lecture 18 Electrochemistry(Concept of Redox reaction, Balancing redox reaction) T-1: Ch 8 Page 330332 Section 8. 2-8. 3 T-2: Ch 19 Page 820 822 Section 19. 1 Week 7 Lecture 19 Electrochemistry(Electrochemical T-1: Ch 8

Page 332cell, Application of electrochemical 335 Section 8. 4 Ch 8 series) Page 335-342 345 347-352 Section 8. 58. 6 8. 8 T-2: Ch 19 Page 823 825 Section 19. 2 Ch 19 Page 827 - 830 Section 19. 3 RW-7 Av33 Week 7 Lecture 20 Electrochemistry (Electrochemical T-1: Ch 8 Page 332cell, Application of electrochemical 335 Section 8. 4 Ch 8 series) Page 335-342 345 347-352 Section 8. 58. 6 8. 8 T-2: Ch 19 Page 823 825 Section 19. 2 Ch 19 Page 827 -830 Section 19. 3 Electrochemistry(Nernst equation, corrosion) T-1: Ch 8 Page 335342 345 347-352 Section 8. 5-8. 6 8. 8 Ch 19 Page 853-854 868 Section 19. 119. 7 T-2: Ch 19 Page 827 830 Section 19. 3 Page 844 - 848 Section 19. 7 T-1: Ch 8 Page 335342 345 347-352 Section 8. 5-8. 6 8. 8 Ch 19 Page 853-854 868 Section 19. 119. 7 T-2: Ch 19 Page 827 830 Section 19. 3 Page 844 - 848 Section 19. 7 RW-7 Galvanic cell Anode cathode Salt bridge and its significance Standard reduction potential and SHE Application of series Analytical numerical To explain how a chemical reaction is used to generate electricity and to provide possible combination of reactants in order to generate electricity Av33 Nernst equation numerical General Type Dry and wet Rusting of iron Corrosion prevention including cathodic protection Nernst equation and To explain deterioration of metals and its prevention Lecture 21 Electrochemistry(Nernst equation, corrosion) Nernst equation numerical General Type Dry and wet Rusting of iron Corrosion prevention including cathodic protection Nernst equation and To explain deterioration of metals and its prevention MID-TERM Week 8 Lecture 22 Acid and bases(Classification of acid-bases, auto ionization of water, pH function, strength of acids and bases) T-2: Ch 15 Page 646 — 652 Section 15. 1 15. 2 15. 3 15. 4 RW-8 Different Concepts Arrhenius Bronsted Lowry and Lewis

Autoionization of Water pH and Its measurement Strength of Acids and Bases Different Concepts Arrhenius Bronsted Lowry and Lewis Autoionization of Water pH and Its measurement Strength of Acids and Bases Equilibrium Involving Weak Acids and base To explain Different Concepts of Acid and bases pH AV 34 35 Lecture 23 Acid and bases(Classification of acid-bases, auto ionization of water, pH function, strength of acids and bases) T-2: Ch 15 Page 646 — 652 Section 15. 1 15. 2 15. 3 15. 4 RW-8 To explain Different Concepts of Acid and bases pH AV 34 35 Lecture 24 Acid and bases(Equilibrium T-2: Ch 15 Page 647— involving weak acids. equilibrium 663 Section 15. 5 15. 6 involving weak bases) Acid base equilibria understanding AV 35 Week 9 Lecture 25 Acid and bases(Equilibrium T-2: Ch 15 Page 647— involving weak acids. equilibrium 663 Section15. 5 15. 6 involving weak bases) Acid and bases(pH of salt solutions, buffers) T-2: Ch 15 Page 674 — 679 Section 15. 10 Ch 16 Page 698 — 716 Section 16. 216. 4 R-1: Ch 6Page259266 T-2: Ch 15 Page 674 — 679 Section 15. 10 Ch 16 Page 698 — 716 Section 16. 216. 4 R-1: Ch 6Page259266 T-2: Ch 16 Page 698 — 716 Section 16. 216. 4 R-1: Ch 7 Page 286314 T-1: Ch 4 Page 165170 Section 4. 5-4. 6 Equilibrium Involving Weak Acids and base pH of salt solutions and buffers Acid base equilibria understanding buffer and salt pH determination AV 35 Lecture 26 AV36 Lecture 27 Acid and bases(pH of salt solutions, buffers) pH of salt solutions and buffers buffer and salt pH determination AV36 Acid and bases(Common ion effect, acid-base titration) Common ion effect and Understanding pH acid base titration curves metric titration ex strong base vs weak acid AV36 Week 10 Lecture 28 Transition Metal Chemistry (Introduction and nomenclature of coordination compounds)

Coordination compounds To explain the basics of AV 37 Ligands Donor atoms metalcomplexes coordination sphere Chelates oxidation state of central metal coordination number Nomenclature examples RW-9 Concept Splitting Energy Factors effecting Splitting Nature of ligands including Spectrochemical series oxidation state of metal and size of d orbitals CFSE in Tetrahedral complexes Splitting in square planar Comparision between Splitting energy of Octahedral and Tetrahedral complexes Effect of geometry on crystal field splitting To define the existence AV 38 39 and stability of different octahedral tetrahedral and square planar complexes of metals Lecture 29 Transition Metal Chemistry (Crystal Field Theory) T-1: Ch 4 Page 155160 Section 4. 2 Week 10 Lecture 30 Transition Metal Chemistry (Crystal Field Theory) T-1: Ch 4 Page 155160 Section 4. 2 RW-9 Concept Splitting Energy Factors effecting Splitting Nature of ligands including Spectrochemical series oxidation state of metal and size of d orbitals CFSE in Tetrahedral complexes Splitting in square planar Comparision between Splitting energy of Octahedral and Tetrahedral complexes Effect of geometry on crystal field splitting Application of crystal field theory in magnetic properties and colour of the complex Application of crystal field theory in magnetic properties and colour of the complex To define the existence AV 38 39 and stability of different octahedral tetrahedral and square planar complexes of metals Week 11 Lecture 31 Transition Metal Chemistry T-1: Ch 4 Page 163(Application of crystal field theory 164 Section 4. 4 in magnetic properties) T-2: Ch 22 Page 950955 Section 22. 5 Transition Metal Chemistry(Colour T-1: Ch 4 Page 163of the complexes) 164 Section 4. 4 T-2: Ch 22 Page 950955 Section 22. 5 To explain the Av 40 properties magnetic

character and colour of metal complexes To explain the AV 40 properties magnetic character and colour of metal complexes Lecture 32 Organometallics(Introductory theory of organometallics and its application) T-1: Ch C Page 187192 Section C. 1 Introduction Example of To explain the basics of Grignard reagent metalcarbon complexes ZeiglerNatta catalyst Application In polymerization with reaction hemoglobin and chlorophyll molecule use of metal in biological system Organometallics(Metals in biology) Lecture 33 Polymerization(Classification of polymers) R-1: Ch 18 page 941945 T-1: Ch 14 Page 601605 Section 14. 114. 2 Terms Monomer To explain different Oligomers Polymers types of polymers polymerization Degree of polymerization Functionality Clasification on the basis of structure types of monomer units Including Types of Copolymers occurance method of synthesis stereochemistry and thermal behavior Uses Addition Condensation and Copolymerisation with examples To provide various Test 2 allotment methods of synthesis of polymers Week 12 Lecture 34 Polymerization(Type of polymerisation) T-1: Ch 14 Page 606607 Section 14. 3 Week 12 Lecture 35 Polymerization(Application of polymers) T-1: Ch 14 Page 601605 634-638 648-649 653-655 Section 14. 1-14. 2 14. 5-14. 6 Application of polymers To provide uses of polymers Lecture 36 Week 13 Lecture 37 Photochemistry(Jablonskii diagram) Photochemistry(Concept of fluorescence) T-1: Ch 22 Page 984986 Section 22. 3 T-1: Ch 22 Page 983989 Section 22. Homework, Test 2 Jablonskii diagram Singlet triplet To explain different possibilities on absorption of radiation Lecture 38 Concept of fluorescence To provide influence of rdiation on behavior of matter phosphorescence Quantum Yield Application of photochemistry in Photovoltaic solar cell To

provide influence of rdiation on behavior of matter To use the principle of photochemistry in Photovoltaic solar cell Photochemistry (Phosphorescence) T-1: Ch 22 Page 987989 Section 22. 5 Lecture 39 Photochemistry (Application of photochemistry in photo voltaic cell /solar cell) T-1: Ch 22 Page 989991 Section 22. 6 SPILL OVER Week 14 Lecture 40 Lecture 41 Revision Revision revision of syllabi upto MTE revision of syllabi after MTE Scheme for CA: Component Homework, Test Frequency 2 Total: Out Of 3 Each Marks Total Marks 10 10 20 20 Details of Academic Task(s) AT No. Objective Topic of the Academic Task Nature of Academic Task (group/individuals/field work Evaluation Mode Allottment / submission Week 2/4 Homework 1 To analyze comprehensive and analytical skills of students Wave-particle duality of light and matter, SchrĶdinger equation, Individual Quantum numbers, Concept of wavefunction and orbitals. Mulitelectron atoms and electron configurations, covalent bonds, ionic bonds (Fajan's rule) and electronegativity concepts, hybridization and shapes of molecules, Molecular orbital theory, molecular orbital diagram for homonuclear diatomic molecule. performance based Homework, Test 1 To analyze the conceptual and analytical skills of students Wave-particle duality of light and matter, SchrÄfÆ'Ä, ¶dinger Individual equation, Quantum numbers, Concept of wavefunction and orbitals, Mulitelectron atoms and electron configurations, covalent bonds, ionic bonds (Fajan's rule) and electro-negativity concepts, hybridization and shapes of molecules, Molecular orbital theory, molecular orbital diagram for homonuclear diatomic molecule. Concept of crystalinity and type of lattices, Band theory and its application in electrical properties of material like conductor, semiconductor and insulator Rate laws, Nuclear

chemistry and elementary reaction, Collision theory, Arhenius concept, Application of Transition state theory (Energy profile diagram), Reaction mechanism. Concept of Redox reaction, Balancing redox reaction Individual Electrochemical cell, Nernst equation, Application of electrochemical series, Corrosion, Classification of Acid-Bases, Autoionization of Water, pH Function, Strength of Acids and Bases, Equilibrium Involving Weak Acids. Equilibrium involving weak bases, pH of salt solutions, and buffers, Common ion effect, Acid-base titration, Introduction of coordination compounds, Nomenclature, Crystal Field Theory and its application. Classification of polymers. Performance based 6/6 Homework, Test 2 To analyze the knowledge of students which they gained from this course. Performance based 11 / 11 Plan for Tutorial: (Please do not use these time slots for syllabus coverage) Tutorial No. Lecture Topic Type of pedagogical tool(s) planned (case analysis, problem solving test, role play, business game etc) Tutorial 1 Importance of chemical principles, Discovery of electron Problem solving and nucleus, Wave-particle duality of light and matter, SchrĶdinger equation, Quantum numbers Concept of wavefunction and orbitals, Mulitelectron atoms and electron configurations, electro-negativity concepts, Periodic properties Problem solving Tutorial 2 Tutorial 3