Lahore University of Management Sciences

CHEM 101 – Principles of Chemistry

Fall 2012

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Course URL (if any)	N/A

Course Basics				
Credit Hours	03			
Lecture(s)	Nbr of Lec(s) Per Week	02	Duration	60 min each
Recitation (per week)	Nbr of Rec (s) Per Week	01 per Section	Duration	60 min each
Lab (if any) per week	Nbr of Session(s) Per Week	N/A	Duration	
Tutorial (per week)	Nbr of Tut(s) Per Week	TBA	Duration	TBA

Course Distribution	
Core	SSE students
Elective	
Open for Student Category	
Closed for Student Category	

COURSE DESCRIPTION

Atomic Structure: General information about the atom and how the theory of the atomic structure evolved. Discovery of electron, Plum pudding model of atom, Rutherford's model of the atom, Max Planck's relationship, emission spectra of atoms and Bohr's theory. Wave-particle duality and De Broglie waves.

Introduction to Quantum Mechanics: Failure of classical mechanics and experiments that led to the development of quantum mechanics. The concept of wavefunction, orbitals and their representation on paper, the radial distribution function, Hydrogen atomic orbitals, quantum numbers, orbitals and energies, Hydrogen like atoms, Multi-electron atoms, concepts of shielding, penetration and effective nuclear charge, Slater's rules, orbital energies of excited states and of empty orbitals and ionization energies.

Electrons in Molecules: Molecular orbitals (MO), linear combination of atomic orbitals, symmetry labels, molecular orbital diagrams, overlap and the overlap integral, H2, He2 and their ions, homonuclear diatomics of the second period, limitations of qualitative MO diagrams, photoelectron spectra, hetronuclear diatomics, hybrid atomic orbitals, sp3 hybrids, sp2 hybrids and sp hybrids, comparing the hybrid and full MO approaches.

Trends in Bonding: Electronic configuration and the periodic table, orbital energies and effective nuclear charges, the second period anomaly, the effects of the d-block, relativistic effects in the heavy elements, electronegativity and orbital energies, atomic sizes across the periodic table, ionization energies and electron affinities, bonding in the non-metals and metals, the transition from metals to non-metals, oxidation states, trends in oxidation states across the periodic table.

Thermodynamics and chemical equilibria: State functions; heat, internal energy and enthalpy; Entropy and second law; Gibbs energy; Chemical equilibrium; standard free change of a chemical reaction;

Acid-Base Equilibria: Classification of acids and bases, acidity and basicity in terms pKa, competition between two acids, leveling effect of solvent, the pH of solutions of weak acids, buffer solutions, acid-base titrations, polyprotic acids.

Chemical Kinetics: The rate of a reaction, rate laws, temperature dependence, the energy barrier to reaction, the transition state, reversible reactions and equilibrium, measuring concentrations, integrated rate laws.

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COURSE PREREQUISITE(S)	
•	None

COURSE OBJECTIVES	
•	• Understand different theories of atomic structure, with special emphasis to quantum mechanics approach and how atomic orbitals combine to form molecules. • Understand the physical meaning of wavefunction and how this can be related to the probability of electron in an atom. • calculate orbital energies of electrons in single and multi-electron atoms • calculate Zeff and its dependence on electron shielding • increase the understanding of the basic concepts in photoelectron spectroscopy, its applications to calculate orbital energies • Understand the bonding, chemical structures and shapes of molecules and trends in bonding across the periodic table. • Discuss acid-base equilibrium and its applications in titrations and buffer solutions. • enhance analytical skills in problem solving capabilities

Learning Outcomes	
•	On completion of this course students should be able to: • Understand the concept of wave function and how it is related to the probability of finding the electron. • Apply quantum mechanics concepts to estimate the energies and shapes of atomic and molecular orbitals. • Apply concept of electron shielding to calculate Zeff. • Calculate orbital energies of both single and multi-electron atoms. • apply photo-electron spectroscopy to find the orbital energies • Draw MO diagrams for homo- and hetro-nuclear diatomic molecules and calculate bond order of these atoms. • use s-p mixing concepts to explain the behavior of diatomic molecules • Correlate physical and chemical properties of elements and molecules to the periodic table. • Understand acid-base equilibria and buffer solutions and perform pH calculations involving these solutions. • Formulate rate equations for simple chemical reactions.

Grading Breakup and Policy
Assignments: 5 % Quizzes: 25 % Mid-term exam: 30 % Final exam: 40 % Instructor has the privilege to change the grading scheme which, if availed, will be conveyed to the students well in time.

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Examination Detail

COURSE OVERVIEW			
Lab experiments	Topics	Recommended Readings	Objectives/ Application
Week 1	Atomic structure	OMC: 1.3, 1.4, 4.1, 4.2, 4.3, 4.4	TBA
Week 2	Introduction to Quantum Mechanics	OMC: 4.5, 5.1, 5.2, 5.3, 5.4 KCS: 2.1, 2.2, 2.3, 2.4, 2.5, 2.6, 2.7	TBA
Week 3	Introduction to Quantum Mechanics	OMC: 4.5, 5.1, 5.2, 5.3, 5.4 KCS: 2.1, 2.2, 2.3, 2.4, 2.5, 2.6, 2.7	TBA
Week 4 - 5	Introduction to Quantum Mechanics	OMC: 4.5, 5.1, 5.2, 5.3, 5.4 KCS: 2.1, 2.2, 2.3, 2.4, 2.5, 2.6, 2.7	TBA
Week 6	Electrons in Molecules	KCS: 3.1, 3.2, 3.3, 3.4, 3.5, 4.3, 4.4, 4.5, 4.6	TBA
Week 7	Trends in Bonding	KCS: 7.1, 7.2, 7.3, 7.4, 7.5, 7.6, 7.7, 7.8, 7.9, 7.10	TBA
Week 8	Trends in Bonding	KCS: 7.1, 7.2, 7.3, 7.4, 7.5, 7.6, 7.7, 7.8, 7.9, 7.10	TBA
Week 9	Thermo and chem. equilibria	OMC: ZCP:	TBA
Week 10	Thermo and chem. equilibria	OMC: ZCP:	TBA
Week 11-12	Acid-Base Equilibria	OMC: 15.1, 15.2, 15.3, 15.4, 15.5, 15.6, 15.7 ZCP:	TBA
Week 13-14	Chemical Kinetics	OMC: 18.1, 18.2, 18.5 KCS: 10.1, 10.2, 10.3, 10.4, 18.1, 18.2	TBA
Midterm Exam	Yes/No: Yes Combine/Separate: Combine Duration: 90 min Preferred Date: During the university mid-term exam week Exam Specifications: Closed books, Course material in any form is not permitted		
Final Exam	Yes/No: Yes Combine/Separate: Combine Duration: 03 h Exam Specifications: Closed books, Course material in any form is not permitted		

Textbook(s)/Supplementary Readings

Textbooks:

James Keeler and Peter Wothers (2008) Chemical structure Reactivity:
An integrated Approach, (1st edition) ISBN: 978-0-19-928930-1 Oxford
David W. Oxtoby, H.P. Gillis and Alan Campion (2008) Principles of modern Chemistry. (6th edition) ISBN: 978-0-534-49366-0 Thomson.
Steven S Zumdahl (2001) Chemical Principles, (6th edition) ISBN: 978-0618946907. Houghton Mifflin