Atoms, Molecules, and Reactions (2011-12)

Expected Syllabus for Quantum Mechanics

Text: Physical Chemistry, 4th Edition by Robert J. Silbey, Robert A. Alberty, Moungi G. Bawendi. Published by John Wiley and Sons copyright July 2004, ©2005; ISBN 978-0-471-21504-2

Chapter	Concepts
9	historical development of quantum mechanics, Black body radiation, Planck's equation, Bohr model, Heisenberg uncertainty principle, Schrodinger equation, Hamiltonian, wavefunction
9	QM operators and their properties, properties of well behaved wavefunctions, postulates of quantum mechanics, expectation value, normalizing a wavefunction, properties of a particle in a one dimensional box
9	properties of a particle in a 3 dimensional box, properties of the harmonic oscillator (classical and quantum mechanical), wavefunction and energy of a quantum mechanical harmonic oscillator, applications to IR spectroscopy
9&10	rigid rotor, angular momentum, spherical polar coordinates, energies and wavefunctions of hydrogen like atoms, spectra of H-like atoms, orbital degeneracy, probability density diagrams
10	Schrodinger equation for H-like atoms, wavefunction for H-like atoms, energy and quantum numbers for H-like atoms, orbital angular momentum, influence of a magnetic field on the Hamiltonian, ladder type energy diagrams, He atom Schrodinger equation and wavefunction, variation theorem, Pauli exclusion principle and its applications, Slater determinants for multi-electron atoms
10&11	Hartree-Fock self consistent field method, periodic trends, aufbau principle, ionization energy, electron affinity, angular momenta and quantum numbers for many electron atoms,atomic term symbols, spin-orbit coupling, atomic spectra and selection rules, Born-Oppenheimer approximation, Schrodinger equation for the hydrogen molecular ion, potential energy diagram
11	wavefunction for the hydrogen molecular ion, Schrodinger equation and wavefunctions for the hydrogen molecule, potential energy diagram for H2, confocal elliptic coordinates, molecular angular momenta and quantum numbers, term symbols for diatomic molecules, hybridization model
11 & 13	Huckel MO theory, Rotational Spectra of diatomic and polyatomic molecules
13	rotational spectra of symmetric tops, vibrational spectra of diatomic molecules, vibration-rotation spectra of diatomic molecules
13 & 14	Raman Spectroscopy (pure rotational and vibration-rotation), Electronic Spectra, Franck-Condon principle, selection rules, fluorescence, phosphorescence, lasers

Expected Syllabus for Inorganic Chemistry

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Chapter	Concepts
Review Chapts. 1, 2, & 3	History of the periodic table, structure of the atom, Bohr model, Heisenberg uncertainty principle, atomic wavefunctions, quantum numbers, radial and angular functions, nodes, aufbau principle, shielding, periodic properties of atoms & ions, Lewis dot structures, resonance, formal charge, expanded valence, VSEPR theory, molecular geometry, electronegativity, bond and molecular polarity, hydrogen bonding, clathrates
4	symmetry operations and elements, symbols for symmetry elements, classification into point groups
4	properties of groups, transformation matrices, matrix and character representations for point groups, character tables, reducible and irreducible representations, applications of symmetry
4 & 5	applications of symmetry (ctd.), MO diagrams of homonuclear diatomics
5	MO diagrams of heteronuclear diatomics, photoelectron spectroscopy and its applications
5	MO diagrams of polyatomic molecules, MO diagrams using hybridization of the central atom
6	Historical development of the definitions of acids and bases, Arrhenius, Bronsted-Lowry, Lewis, Solvent System, and Frontier Orbital concepts of acids and bases, hard and soft acids/bases, measuring acid/base strengths, inductive solvent, and steric effects on acid/base strengths, strength of oxyacids, acid/base strength in non-aqueous solvents
7	coordination numbers, lattice points, unit cell, closest packing, simple crystal structures
7	Bravais lattices, groupings of crystalline solids (metals, alloys, ionics), energetics of crystal formation, Born-Haber cycle, lattice enthalpy
7	band theory of solids applied to metals, semi-metals, semiconductors, and superconductors and the effect of temperature on their conductivity
9 & 10	isomerism in coordination compounds, valence bond theory, crystal field theory and ligand field theory to understand bonding in coordination compounds
10	molecular orbital diagrams to show sigma and pi bonding in octahedral and tetrahedral complexes, ligand flied stabilization energy of high spin-low spin complexes, spectrochemical series, Lewis pi acids and bases, magnetic susceptibility measurements
10 & 11	tetragonal distortions, Jahn-Teller effect, MO diagrams for square planer complexes, Correlation Diagrams, Tanabe-Sugano diagrams
11	Correlating Tanabe-Sugano diagrams with the electronic spectra of octahedral and tetrahedral transition metal complexes, determining octahedral splitting energy from spectra, charge transfer spectra