

M. Sc. Semester -I

CHE401 Inorganic Chemistry

Unit 1 -Quantum theory and Atomic Structure

Postulates of quantum mechanics, setting up of different observables, eigen value of angular momenta and commutation relations, step-up and step-down operators, angular momenta in many electron atoms.

Schrodinger wave equation and applications : particle on a ring and the simple harmonic oscillator.

H-atom wave functions, solutions of $R(r)$, $\theta(\theta)$ and $\phi(\phi)$ equations, quantum numbers, angular and radial wave function, shapes of the orbitals, angular momentum of inner quantum number j , physical interpretation of hydrogenic orbitals; space quantization of electronic orbits; electron spin.

Approximation methods : Variation method and application to H atom. Perturbation theory (first order and non-degenerate, application to the Helium atom)

Unit 2- Symmetry and Group Theory

Representation of groups –some properties of matrices & vectors, representation of groups, the Great orthogonality theorem and its consequences, character table, wave functions as basis for irreducible representations, direct product, identifying non-zero matrix elements.

Unit 3- Magnetochemistry

Magnetic susceptibility and basic derivation of diamagnetic susceptibility, pascal constant and its utility, Curie law and Curie-Weiss law, antiferromagnetism and ferromagnetism. Types of antiferromagnetism, antiferromagnetic exchange pathway :

Direct –metal- metal interaction and Indirect-atom exchange i.e. super exchange mechanism.

Unit 4- Bio-inorganic Chemistry

Metalloporphyrins (enzymes) definition, hemoglobin and myoglobin, cytochrome, vitamin B₁₂ (cyano cobalamin), zinc metallo enzymes, nitrogen fixation, essential and trace elements in biological system, biochemistry of non metals K, Na pump (action of bath ions), toxic metals and their toxicity.

Co-ordination compounds in medicine

Chelation therapy, gold compounds and rheumatoid arthritis, anticancer drugs –platinum complexes, gold complexes, metallocenes etc, antimicrobial agents, metal complexes as radiodiagnostic agents, magnetic resonance imaging.

CHE401 Inorganic Chemistry

Semester I – Theory

References:

1. Introduction to Quantum Chemistry, A. K. Chandra, Tata MacGraw Hill
2. Quantum Chemistry, Ira N. Levine, Prentice Hall
3. Quantum Chemistry by R. K. Prasad, New Age International Publishers (1985)
4. Elementary Quantum Chemistry by D. L. Pilar, Mc Graw Hill Book Co, New York (1968)
5. D. A. McQuarrie Quantum Chemistry, OUP 1983
6. M. W. Hanna, Quantum Mechanics in Chemistry, The Benjamin Pub.
7. Molecular Quantum Mechanics, Third Edition, P. W. Atkins and R.S. Friedman
8. Group theory and symmetry in chemistry, L. H. Hall(McGraw Hill)
9. F. A. Cotton, Chemical Applications of Group theory, Wiley Eastern 2nd Edn.1992
10. V. Ramkrishnan & M. S. Gopinadhan, Group theory in Chemistry Vishal Pub.1996.
11. Inorganic Chemistry, Third Edition, Alan G. Sharpe
12. Theoretical Inorganic Chemistry, M. C. Day, J. Shellin
13. Chemistry, Fifth Edition, John E. McMurry, Robert C. Fay
14. Hermann Dugas, Bioorganic Chemistry, A Chemical Approach to Enzyme Action, Springer International Edition
15. An Introduction to Theoretical Chemistry, Jack Simons, Cambridge
16. Progress in inorganic Chemistry, Vols 18 and 38 ed. J. J. Lippard, Wiley
17. Inorganic Reaction Mechanisms, M. L. Tobe, Nelson Pub
18. Inorganic Chemistry, K. F. Purcell and J. C. Kotz.
19. Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Bers
20. Bioinorganic Chemistry, I. Bertini, H. B. Gray and S. J. Lippard
21. Principals of Bioorganic Chemistry, S. J. Lippard and J. M. Berg, University Science Books.
22. Bioinorganic Chemistry, I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, University Science Books.
23. Inorganic Biochemistry vols I and II ed. G. L. Eichhorn, Elsevier
24. Introduction to Magnetochemistry, Alan Earnshaw, 1968
25. Elements of Magnetochemistry, Dutta and Syamal, 1993

M. Sc. Semester I- Practicals
CHE405PR Inorganic Chemistry

Semester –I Practicals (Inorganic Chemistry) CHE405PR

1. Semi-microqualitative analysis of 15 mixtures, each having six radicals including less familiar elements (Mo, W, Li, Th, V, Zr, Ce, Be, Ti) and one insoluble compounds.

M. Sc. Semester I- Practicals
CHE405PR Inorganic Chemistry

References

1. Vogel's Qualitative Inorganic Analysis, Revised by G Svehla, Sixth Edition, Longman, 1987

M. Sc. Semester II

Inorganic Chemistry-CHE407

Unit I- Chemical Bonding

The method of linear combination

VSEPR, Walsh diagrams(tri-and penta- atomic molecules), $d_{\pi}-p_{\pi}$ bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

Simple Huckel theory of linear conjugated systems, simple Huckel theory of the cyclic conjugated system and aromaticity, self consistent field method, valence state ionization potentials, Pariser-Parr-Pople approximation.

Band theory of solids, Fermi level, electrical properties, insulators, semiconductors and superconductors (properties).

Unit 2- Application of symmetry

Application of symmetry to hybrid orbital, molecular orbitals, hybridization schemes for σ orbitals, π bonding and molecular orbital for AB_n type of molecules.

Application of symmetry to molecular vibrations, interpretation of IR and Raman spectral data.

Unit 3-Organometallic Compounds

Organometallic compounds of transition elements, stability of metal carbon bond in complexes. Synthesis, uses and structure of organometallic compounds of π bonding organic ligands, 2-electron ligands, olefinic and acetylinic complexes, compound with 3 electron ligand – allylic complexes, compounds. With 4- electron ligands butadiene complexes, n^4 complexes of cyclopentadiene, compounds with 5 electron ligands – cyclopentadienyl, compounds with 6 electron ligands, n^6 complexes of benzene and its derivatives.

Role of organometallic compounds in catalytic reaction.

Unit 4 – Reaction Mechanism

Mechanism of substitution reaction in square planar complexes. Kinetics of substitution reaction of platinum (II) complexes

Effect of leaving group, effect of charge, steric effect, solvent effect, effect of nucleophile, effect of temperature and other effects.

Oxidation-Reduction reaction, electron transfer, tunnelling effect, Marcus –Hush theory, one and two electron transfer inner sphere and outer sphere, effect of ions on rate, electron transfer through extended bridges, unstable oxidation states, hydrated electron.

M. Sc. Semester –II
CHE407 (Inorganic Chemistry)- Theory

References

1. Introduction to Quantum Chemistry, A. K. Chandra, Tata MacGraw Hill
2. Quantum Chemistry, Ira N. Levine, Prentice Hall
3. Quantum Chemistry by R. K. Prasad, New Age International Publishers (1985)
4. D. A. McQuarrie Quantum Chemistry, OUP 1983
5. M. W. Hanna, Quantum Mechanics in Chemistry, The Benjamin Pub.
6. Lectures on Chemical Bonding and Quantum Chemistry, S. N. Datta, A Prism Book
7. Group theory and symmetry in chemistry, L. H. Hall(McGraw Hill)
8. Coulson's Valence, R. McWeeny, ELBS
9. F. A. Cotton, Chemical Applications of Group theory, Wiley Eastern 2nd Edn.1992
10. V. Ramkrishnan & M. S. Gopinadhan, Group theory in Chemistry Vishal Pub.1996.
11. Inorganic Chemistry, Third Edition, Alan G. Sharpe
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13. Chemistry, Fifth Edition, John E. McMurry, Robert C. Fay
14. An Introduction to Theoretical Chemistry, Jack Simons, Cambridge
15. Progress in inorganic Chemistry, Vols 18 and 38 ed. J. J. Lippard, Wiley
16. Mechanism of Inorganic Reactions, F. Basolo and R. G. Persons, Wiley Pub
17. Reaction Mechanism of Coordination Compounds, C. H. Langford and H. B. Gray
18. Inorganic Reaction Mechanisms, M. L. Tobe, Nelson Pub
19. Inorganic Chemistry, K. F. Purcell and J. C. Kotz.
20. Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Bers
21. Mehrotra R. C. and Singh A. Organo Metallic Chemistry, Willey Eastern Ltd., New Delhi
22. Coates G. E. Green MIH Wade, K and Aylett B. J. Organo Metallic Comounds Chapman and Hall, London

M. Sc. Semester II- Practicals

CHE411PR (Inorganic Chemistry)

Semester –II Practicals (Inorganic Chemistry) CHE411PR

1. Preparation and determination of purity of double and complex salts. At least ten preparations should be done.
2. Colourimetric estimation of any five out of Cu, Mn, NO₂, Ni, P, Fe, V, Ti, Cr, Co.

M. Sc. Semester II- Practicals

CHE411PR (Inorganic Chemistry)

References

1. Vogels Textbook of Quantitative Chemical Analysis, 6th Edition, 2002.
2. Advanced Practical Inorganic Chemistry, Gurdeepraj, Goel Publishing House, 2001.
3. An Advanced Course in Practical Chemistry, A.K. Nad, B. Mahapatra, A. Ghosal, New Central Book Agency, 2004