



PROGRAMS AND BIBLIOGRAPHY

Subject	
Code	Name
QI242	Theoretical Inorganic Chemistry

Vector
OF:S-2 T:004 P:000 L:000 O:000 D:000 HS:004 SL:004 C:004 AV:N EX:S FM:75%

Pre requirement
QG101 QG102/QG108 QG109

Summary
Atomic Structure. Periodicity. Chemical Bonding Models. Acidity and Basicity. Coordination Compounds. Introduction to Organometallic Compounds and Catalysis.

Program
Atomic Structure and Periodic Table (Revision) Chemical Bonding Models Diagram of potential energy versus internuclear distance between two hydrogen atoms. Ionic bonding and lattice energy. Covalent bonding. Concepts of Polarizability and Electronegativity. Molecular Orbital Theory. Secondary bonding. Metallic bonding. Band theory and introduction to conductor, semiconductor and insulating materials. Introduction to Solid State Chemistry Unit cells. Bravais lattice and the concept of close packing of atoms. Tetrahedral and octahedral interstitials and the idea of atomic blends. Introduction to the X-ray diffraction technique. Acids and Bases Definition of Lewis acids and bases. Hard soft acid base theory and its usefulness. Coordination Chemistry Definition of coordination compounds. Chelate effect. Structural Isomers and stereoisomers. Crystal field theory. Ligand field theory. Jahn-Teller effect. Reactivity of coordination compounds; Mechanisms of ligand substitution reactions; The trans effect; Mechanisms of redox reactions. Introduction to Organometallic Chemistry and Catalysis Concepts, definitions and usual ligands (M-CO and M-PR ₃). The eighteen-electron rule. Thermodynamic and kinetic parameters of substitution, oxidative addition and reductive elimination reaction mechanisms. Presentation of some organometallic catalytic cycles and their importance in commercial processes.

Bibliography

Textbooks

D. F. Shriver, P. W. Atkins, C.H. Langford. Inorganic Chemistry. 2nd. ed. Oxford : Oxford University Press, 1994. 819p.

J. E. Huheey, E. A. Keiter, R. L. Keiter. Inorganic Chemistry: Principles of Structure and Reactivity. 4th ed. New York : Harper Collins, 1993. 964p.

Supplemental Readings

G. L. Miessler, D. A. Tarr. Inorganic Chemistry. 4th ed., Harlow : Pearson, 2011. 1213p.

C. E. Housecroft, A. G. Sharpe. Inorganic Chemistry. 4th ed. Upper Saddle River. NJ : Prentice-Hall, 2012. 754p.

Evaluation criteria

For grading policy, see: Regimento Geral de Graduação, Seção I – Normas Gerais, Capítulo V – Da Avaliação do Aluno na Disciplina. Students are required to attend 75 % of the lectures.

For further details, see: Regimento Geral de Graduação, capítulo VI, seção X, artigo 72.