Code: **QI242**

Nome: **Química Inorgânica Teórica**

Nome em Inglês: **Inorganic Theoretical Chemistry**

Nome em Espanhol: **Química Inorgánica Teórica**

Subject type: **Semesterly**

Approval type: **Grade and Attendance**

Characteristic: **Regular**

Frequency: **75%**

Period Type / Offering period: **Semesterly / All terms**

Requires Final Exam: **Yes**

Vectors

T	L	P	O	PE	OE	SL	WEEKS	CREDIT
4	**-**	**-**	**-**	**-**	**-**	**4**	**15**	**4**

Occurrence on curriculum: **09, 39, 63**

Pre requirement:

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

Basic Bibliography

1) SHRIVER, D. F.; ATKINS, P. W.; LANGFORD, C.H. **Inorganic Chemistry**. 2nd. ed. Oxford: Oxford University Press, 1994.

2) HUHEEY, J. E.; KEITER, E. A.; KEITER, R. L. **Inorganic Chemistry: Principles of Structure and Reactivity.** 4th ed. New York Harper Collins, 1993.

3) ATKINS, P.; JONES, L.; LAVERMAN, L. **Princípios de Química: questionando a vida moderna e o meio ambiente**, 7th ed. Bookman, 2018.

Supplementary Bibliography

1) MIESSLER, G. L.; TARR, D. A. **Inorganic Chemistry.** 4th ed., Harlow: Pearson, 2011.
2) HOUSECROFT, C. E.; SHARPE, A. G. **Inorganic Chemistry**. 4th ed. Upper Saddle River. NJ: Prentice-Hall, 2012.
3) RUSSEL, J. B. **Química Geral**, volumes 1 e 2. 2ª ed. Pearson, 2006.
4) BROWN, T. L.; LEMAY, H.E.; BURSTEN, B. E.; BURDGE, J.R. **Química a Ciência Central**. 13ª ed. Pearson, 2016.
5) CALLISTER-JR, W. D.; RETHWISH, D. G. **Fundamentos da Ciência e Engenharia de Materiais: uma introdução**, 8ª Ed. LTC, 2012.