

## SYLLABUS

# ANALYTICAL CHEMISTRY

### ANALYTICAL ASPECTS OF ELECTRO ANALYTICAL CHEMISTRY 1

#### Syllabus:

1. Historical aspects, classification of electro analytical techniques and review of concepts of electrolytic and non-electrolytic cells (galvanic).
2. Principles of Conventional Polarography (DC): Circuit and polarography cells; dropping mercury electrode; Electrolyte support; Removal of oxygen; Scope of polarography; Limits of diffusion, residual and migration currents; Ilkovic equation; Polarography AC, Tast (sampling), normal pulse and differential pulse.
3. Voltammetria cíclica (CV: Cyclic voltammetry).
4. Chronoamperometry.
5. Voltammetria de varredura linear (LSV: linear sweep voltammetry).
6. Experiments demonstrating some techniques and applications of environmental, biological, pharmaceutical and industrial interest.
7. Seminars.
8. List of exercises.
9. Tests.
10. International Journals Papers.

#### References:

- 1- Bard, A.J. and Faulkner, L. R., "Electrochemical Methods: Fundamentals and Applications", 2nd ed., John Wiley, New York, 2001.
- 2- Bond, A.M. and Foulkner, L.R., "Electrochemical Methods Fundamentals and Applications", John Wiley & Sons, New York, 1980.
- 3- Kolthoff, I.M. and Lingane, J.J., "Polarography", 2nd ed., Interscience Publ., New York, 1952.

### ANALYTICAL ASPECTS OF ELECTROANALYTICAL CHEMISTRY 2

#### Syllabus:

1. Introduction.
2. NPV: normal pulse voltammetry.
3. DPV: differential pulse voltammetry.
4. SWV: square wave voltammetry.
5. ASV: anodic stripping voltammetry.
6. CSV: cathodic stripping voltammetry.
8. AdSV: adsorptive stripping voltammetry.
9. Experiments demonstrating some techniques and applications of environmental, biological, pharmaceutical and industrial interest.
10. Seminars.
11. List of exercises.
12. Tests.

#### References

- 1- Bard, A.J. and Faulkner, L. R., "Electrochemical Methods: Fundamentals and Applications", 2nd ed., John Wiley, New York, 2001

- 2- Kolthoff, I.M. and Lingane, J.J., "Polarography", 2nd ed., Interscience Publ., New York, 1952.
- 3- Giolito, I., "Métodos Eletrométricos e Eletroanalíticos: Fundamentos e Aplicações", 2a ed., Multitec, São Paulo, 1980.

## **CONTINUOUS FLOW ANALYSIS**

### **Syllabus**

1. Introduction.
2. Non-segmented flow analysis.
3. Components of flow injection systems.
4. Projects of flow injection systems.
5. Segmented streaming analysis.
6. Kinetic aspects in flow systems.
7. Analytical applications and trends.
8. Seminars.

### **References**

- 1- A. Sanz-Medel, ed. "Flow Analysis with Atomic Spectrometric Detectors". Elsevier, Amsterdam, 1999.
- 2- M. Trojanowicz. "Flow Injection Analysis. Instrumentation and Applications". World Scientific Publishing, Singapore, 2000.
- 3- M. Valcárcel, M.D. Luque de Castro e A. Losada. "Flow Injection Analysis: Principles and Applications". Ellis Horwood, 1987.

## **ANALYTICAL ASPECTS OF CHEMICAL SOLUTIONS**

### **Syllabus**

1. Introduction.
2. Balance constants. Activity.
3. Thermodynamic aspects of equilibrium.
4. Simultaneous equilibria.
5. Equilibria and titration curves.
6. Determination of equilibrium constants. Typical systems. Computer Algorithms.
7. Seminars.
8. International Journals Papers.

### **References**

- 1- A.J. Bard. "Chemical Equilibrium". Harper & Row, 1976.
- 2- A.E Martell e R.J. Motekaitis. "Determination and Use of Stability Constants". VCH, 1988.
- 3- M. Meloun, J.Havel e E. Hogfelf. "Computation of Solution Equilibria: A Guide to Methods of Potentiometry, Extraction and Espectrophotometry". Ellis Harwood, 1988.

## **ENVIRONMENTAL CHEMISTRY 1**

### **Syllabus**

1. Biogeochemical cycles of the elements.
2. Chemical processes in the atmosphere.
3. Hydrochemical soil and the lithosphere.
4. Chemical processes in aquatic systems.
5. Environmental chemistry and energy sources.

6. Environmental Impact Assessment.
7. Treatment of waste and effluents.
8. Environmental legislation (water, soils and atmosphere).
9. Fundamentals of Ecotoxicology.
10. International Journals Papers.

### References

- 1- S.E. Manahan. "Environmental Chemistry", 6a ed. CRC Press, 1994.
- 2- C. Baird. "Environmental Chemistry". W.H. Freeman, 1994.
- 3- R.N. Reeve e J.D. Barnes (Ed.). "Environmental Analysis (Analytical Chemistry by Open Learning)". John Wiley & Sons, 1994.

## CHEMICAL SENSORS

### Syllabus

1. Introduction.
2. Theoretical foundations.
3. Performance of chemical sensors.
4. Potentiometric Sensors.
5. Amperometric Sensors.
6. Piezoelectric sensors.
7. Fiber Optic Sensors.
8. Other Sensors.
9. Construction, evaluation and analytical techniques using chemical sensors.
10. Seminars.
11. Recent Papers.

### References

- 1- U. Spichiger-Keller. "Chemical Sensors and Biosensors for Medical and Biological Applications". VCH, 1998.
- 2- R.W. Cattrall. "Chemical Sensors (Oxford Chemistry Primers, 52)". Oxford University Press, Oxford, 1997.
- 3- R. Freitag, "Biosensors in Analytical Biotechnology", Academic Press, Austin, 1996.

## OPTICAL METHODS APPLIED TO TRACE DETERMINATION

### Syllabus

1. Introduction.
2. Atomic absorption spectrophotometry with electro thermal atomization.
3. Atomic absorption spectrophotometry: generation of hydrides and cold vapor.
4. Induced plasma atomic emission spectrometry (ICP-AES).
5. Plasma spectrometry coupled to mass spectrometry (ICP-MS).
6. Hyphenated techniques.
7. Chemical Speciation.

### References

- 1- A.G. Howard e P.J. Statham. "Inorganic Trace Analysis - Philosophy and Practice". Chichester, John Wiley & Sons, 1993.
- 2- Vandecasteele e C.B. Block. "Modern Methods for Trace Element Determination". Chichester, John Wiley & Sons, 1993.

- 3- R. Cornelis, J. Caruso, H. Crews, K. Heumann, eds. "Handbook of Elemental Speciation. Techniques and Methodology. John Wiley, 2003.

## **ANALYTICAL CHEMISTRY TOPICS**

**Syllabus and References are changeable.**

## **PHYSICAL CHEMISTRY**

### **CHEMICAL KINETICS**

#### **SYLLABUS**

1. Kinetic theory of gases.
2. Transportation by diffusion.
3. Speed of simple chemical reactions and mechanisms.
4. Mechanism of complex chemical reactions.
5. Molecular dynamics.
6. Reactions in Solution Reactions Solution.
7. Catalysis.
8. Solid state reactions.

#### **REFERENCES**

1. Laidler, K.J. "Theories of Chemical Kinetics" New York, McGraw-Hill, 1969.
2. Atkins, P.W. "Physical Chemistry", 5<sup>a</sup> ed. Oxford University Press, 1994.
3. Levide D. "Molecular Reaction Dynamics" Cambridge University Press, 2005

### **QUANTUM CHEMISTRY 1**

#### **SYLLABUS**

1. Origins of the quantum theory.
2. Wave functions, operators, matrices and the uncertainty principle.
3. Quantum theory for some simple systems: free particle, in the box, etc.
4. Interaction of radiation with matter.
5. Angular momentum in quantum mechanics.
6. Hydrogen atom.
7. Methods of approach in quantum mechanics.
8. Poly electronic atoms: electronic wave functions; Spin; Princ. de Pauli, etc.
9. Introduction to molecular structure.
10. Electronic structure of molecules: H<sub>2</sub> + molecules, etc.

#### **REFERENCES**

1. Ira N. Levine. "Quantum Chemistry", 5<sup>a</sup> ed. Allyn and Bacon, 1999.
2. P.W. Atkins. "Molecular Quantum Mechanics", 2<sup>a</sup> ed. Oxford University Press, 1983.
3. Donald A. McQuarrie "Quantum Chemistry" University Science Books, 1983.

### **CHEMICAL THERMODYNAMICS**

#### **SYLLABUS**

1. First Law of Thermodynamics.
2. Applications of the first law.
3. Second law of thermodynamics.

4. Applications of the second law.
5. Thermodynamic functions for pure substances. Physical equilibria.
6. Thermodynamic functions for mixtures. Physical equilibria.
7. The rule of phases and their applications.
8. Thermodynamic functions for chemical equilibria.
9. Thermodynamics of ions.

## REFERENCES

- 1- G.N. Levis e M. Randall (edição revisada por K.S. Pitzer e L. Brewer). "Thermodynamics". Mc-Graw Hill, 1961.
- 2- P.W. Atkins. "Physical Chemistry", 5a ed. Oxford University Press, 1994.
- 3- A.N. Adamson "A textbook of physical chemistry" 2ª ed. Academic Press, 1979.

## STATISTICAL THERMODYNAMICS

### SYLLABUS

1. Canonical "Ensemble" and fluctuations.
2. Introduction to statistical methods.
3. Classical statistical mechanics.
4. Ideal monatomic gases.
5. Ideal polyatomic gases.
6. Chemical equilibrium.
7. Introduction to quantum statistical mechanics.
8. Partition Functions.

### REFERENCES

- 1- D.A. McQuarrie "Statistical Thermodynamics" Harper & Row, 1973.
- 2- A.N. Matveev "Molecular Physics" Mir Publishers, 1985.
- 3- A. Maczek "Statistical Thermodynamics" Oxford University Press, 1998.

## ADVANCED ELECTROCHEMISTRY

### SYLLABUS

1. Introduction.
2. Electrochemistry of solutions.
3. Electrode-solution interface.
4. Kinetics of electrochemical reactions on inert electrodes. Electrochemical reactions in solution.
5. Kinetics of electrochemical reactions on active electrodes.
6. Electrochemistry of semiconductors.
7. Special techniques in electrochemistry (optical techniques, X-ray diffraction, impedance, etc.).

### REFERENCES

- 1- A.J. Bard e L.R. Faulkner. "Electrochemical Methods". John Wiley and Sons, 1980.
- 2- K.B. Oldham e J.C. Myland. "Fundamentals of Electrochemical Science". Academic Press, 1994.
- 3- J.O.M. Bockvis e A.K.N. Reddy. "Modern Electrochemistry", Vol.I. Plenum Press, 1978.

## CORROSION FUNDAMENTALS

### SYLLABUS

1. Pourbaix diagrams and electrochemical kinetics.
2. Kinetics of dissolution of metals.
3. Kinetics of formation of films on metals.
4. Properties of metal / film / solution systems.
5. Kinetics of hydrogen formation.
6. Oxygen reduction kinetics.
7. Table of mixed potentials.

### REFERENCES

- 1- A.J. Bard e L.R. Faulkner "Electrochemical Methods. Fundamentals and Applications". John Wiley & Sons, 1980.
- 2- Norio Sato "Electrochemistry at Metal and Semiconductor Electrodes" Elsevier, 1998.
- 3- H.B. Ives, J.L. Luo e J.R. Rodda "Passivity of Metals and Semiconductors". The Electrochemical Soc. Inc., 2001.

## QUANTUM CHEMISTRY 2

### SYLLABUS

1. Poly electronic atoms.
2. Hartree-Fock Methods.
3. More sophisticated methods than Hartree-Fock.
4. Introduction to diatomic molecules.
5. Valence bond theory.
6. Molecular orbital methods.
7. Methods of configuring interactions and MCSCF for molecular calculations.
8. Atomic and molecular spectroscopy.

### REFERENCES

- 1- E.R. Davidson and B. Feller "Basis Set Selection in Molecular Calculations". Che. Rev. 1986.
- 2- A. Szabo e N.S. Ostlund. "Modern Quantum Chemistry". Macmillan, 1982.
- 3- H.F. Schaefer III, "The Development of Ab Initio Methods in Molecular Electronic Structure Theory". Oxford University Press, 1984.

## PHYSICAL CHEMISTRY TOPICS

Syllabus and References are changeable.

## CHEMISTRY

### METHODOLOGY OF EDUCATION IN CHEMISTRY

#### SYLLABUS

1. Teaching chemistry with Brazilian legislation.
2. Objectives and methods of teaching chemistry at the high school and college courses.
3. The main references on education in chemistry: main aspects.
4. Main approaches to theoretical and experimental teaching in chemistry.

5. Educational resources for teaching chemistry.
6. Structured investigative approach in the teaching-learning process of chemistry.
7. Main research topics in Chemistry education.

## REFERENCES

1. Castanho, S. e Castanho, M.E. (orgs) "Temas e Textos em Metodologia do Ensino Superior". Papyrus editora, 2001.
2. Souza, P.N.P. "LDB e Educação Superior: Estrutura e Funcionamento". 2ª ed. Pioneira Thomson Learnig, 2001.
3. Junior, J.R.S. e Sguissardi, V. "Novas Faces da Educação Superior no Brasil". 2ª ed. Cortez Editora, 2001.

## TOPICS IN CHEMISTRY

**Syllabus and References are changeable.**

## INORGANIC CHEMISTRY

### ADVANCED INORGANIC CHEMISTRY

#### SYLLABUS

1. Atoms and molecules.
2. Chemical bonding.
3. Properties of elements based on periodic classification.
4. Acids and bases.
5. Coordination compounds.
6. Theory of the crystalline field and molecular orbitals.
7. Organometallic compounds.
8. Coordination compounds in biological systems.

#### REFERENCES

1. D.F. Shriver, P.W. Atkins "Química Inorgânica", 3a ed. Trad. Maria Aparecida Gomes, Porto Alegre, 2003.
2. G.E. Rodgers. Introduction to Coordination, Solid State, and Descriptive Inorganic Chemistry?. McGraw Hill, 1994.
4. K.M. MacKay, R.A. MacKay e W. Henderson. Introduction to Modern Inorganic Chemistry?, 5a ed. Chapman & Hall, 1996.
5. B.E. Douglas, D.H. McDaniel e J.J. Alexander. Concepts and Models of Inorganic Chemistry?, 3a ed. Wiley, 1994.

## PHYSICAL METHODS IN INORGANIC CHEMISTRY

### SYLLABUS

1. Theory of groups applied to molecular symmetry.
2. Vibrational-IR and Raman-laser spectroscopy.
3. Electron-visible and UV spectroscopy.
4. Nuclear magnetic resonance spectroscopy.
5. Crystallographic techniques.
6. Electrochemical techniques.
7. Electron paramagnetic resonance.

### REFERENCES

1. E.A.V. Ebsworth, D.W.H. Rankin e S. Craddock. "Structural Methods in Inorganic Chemistry", 2a ed. Blackwell Scientific, 1991.
2. K. Nakamoto. "Infrared and Raman Spectra of Inorganic and Coordination Compounds", 5a ed. John Wiley & Sons, 19897.
3. R.S. Drago. "Physical Methods for Chemistry", 2a ed. Saunders College Publishing, 1992.
4. J.K.M. Sanders e B.K. Hunter Modern NMR Spectroscopy Oxford University Press. Oxford, 1997.

## HOMOGENEOUS CATALYSIS

### SYLLABUS

1. Introduction.
2. The chemistry of transition metals relevant to catalysis.
3. Carbon monoxide reactions.
4. Reactions of organic substrates.
5. Oxidation of hydrocarbons by oxygen.
6. Ziegler type catalysts.
7. Asymmetric Synthesis.

### REFERENCES

1. Ojima "Catalytic Asymmetric Synthesis" VCH, 1993.
2. J. Reedijk (Ed) "Bioinorganic Catalysis". Marcel Dekker, 1993.

## HETEROGENEOUS CATALYSIS

### SYLLABUS

1. Introduction to heterogeneous catalysis.
2. Physic-chemical adsorption.
3. Properties of the catalysts.
4. Preparation of catalysts.
5. Physic-chemical characterization of catalysts.
6. Metal catalysts, acid-base and ions on the surface of catalysts.
7. Materials used as catalysts.
8. Measures of activity and selectivity.

### REFERENCES

1. J.L. Figueredo e F. Ramôa Ribeiro. "Catálise Heterogênea". Fundação Calouste Gulbenkian, Lisboa, 1989.
2. G.A. Somorjai. "Introduction to Surface Chemistry and Catalysis". John Wiley & Sons, New York, 1994.



3. M. Bowker "The Basis and Applications of Heterogeneous Catalysis" Oxford Science Publications, Series sponsor ZENECA, New York, 1998.
4. J.W. Niemantsverdriet. "Spectroscopy in Catalysis. Na Introduction". VCH, 1995.
5. B.C. Gates. "Catalytic Chemistry". John Wiley and Sons, 1992

## CHEMISTRY OF COORDINATION

### SYLLABUS

1. Review of fundamental theories in inorganic chemistry.
2. Nomenclature, isomerism.
3. Thermodynamic and kinetic stability of complexes.
4. Binders; Coordinate number and geometry of the complexes.
5. Addition, substitution and redox reactions in coordination compounds.
6. Organometallic compounds.

### REFERENCES

1. F.A. Cotton e G. Wilkinson. "Advanced Inorganic Chemistry", 6a ed. Wiley Interscience, 1999.
2. J. Dupont "Química Organometálica, elemento do bloco d" Porto Alegre, 2005.
3. C.J. Jones "A Química dos Elementos dos Blocos D e F" Trad. Maria D. Vargas, Porto Alegre - RS, Artmed Editora, 2002

## MECHANISM AND KINETICS OF INORGANIC REACTIONS

### SYLLABUS

1. Theory of the coordinated connection.
2. Stability of metal complexes.
3. Reactions in non-aqueous solvent.
4. Replacement reactions in octahedral complexes.
5. Stereo chemical changes in octahedral complexes.
6. Replacement reactions in flat square complexes.
7. Oxidation-reduction reactions.
8. Reaction of organometallic compounds of transition metals.

### REFERENCES

1. E.C. Constable. Metals and Ligand Reactivity: An Introduction to the Organic Chemistry of Metal Complexes?, ed. rev. VCH, 1995.
2. W.W. Porterfield. Inorganic Chemistry: A Unified Approach? 2a ed. Academic Press, 1993.
3. S. Asperger "Chemical Kinetics and Inorganic Reaction Mechanisms" Springer, 2003.

## INORGANIC CHEMISTRY IN BIOLOGICAL SYSTEMS

### SYLLABUS

1. Introduction.
2. Biologically important compounds.
3. Coordination chemistry fundamentals.
4. Metals in biological systems.
5. Porphyrin systems and heme proteins.
6. Non-heme proteins.
7. Model systems.
8. Toxicity of individual elements.

## REFERENCES

1. L.R. Milgrom "The Colours of life: An introduction to the chemistry porphyrins and related compounds" oxford university press, 1997.
2. S.J. Lippard e J.M. Berg. Principles of Bioinorganic Chemistry? University Science Books, 1996.
3. N. Farrel, "Transition Metal Complexes as drugs and Chemotherapeutic Agents (Catalysis by Metal Complexes, vol. 11) Kluwer Academic, 1990"

## CRYSTAL PHYSICS

### SYLLABUS

1. Elements of symmetry Production and properties of X-rays.
2. X-ray diffraction techniques of diffraction and interpretation of data.
3. Production and properties of synchrotron radiation.
4. Applications of synchrotron radiation in the characterization and study of condensed materials.

### REFERENCES

1. B.D. Cullity. Elements of X-Ray Diffraction? 2a ed. Addison Wesley, 1988.
2. G. Margaritondo. Introduction to Synchrotron Radiation? Oxford University Press, 1988.
3. B.K. Agarwal. X-Ray Spectroscopy: An Introduction (Springer Series in Optical Sciences, Vol 15)?, 2a ed. Springer-Verlag TELOS, 1991.
4. Fundamentals of Crystallography Ed. by Carmelo Giacovazzo Oxford Science Publication, 1996

## TOPICS IN INORGANIC CHEMISTRY

Syllabus and References are changeable.

## ORGANIC CHEMISTRY

### ADVANCED ORGANIC CHEMISTRY

#### SYLLABUS

1. Chemical bond and structural theory.
2. Acids, bases and catalysis.
3. Reactivity and structure.
4. Stereochemistry and Conformational Analysis.
5. The rules of Woodward-Hoffmann.
6. Photochemistry.
7. The reactive intermediates.

#### REFERENCES

- 1- F.A. Carey e R.J. Sundberg "Advanced Organic Chemistry", 4<sup>a</sup> ed. Kluwer Academic/Plenum Publishers, 2001.
- 2- J. Clayden, N. Greeves, S. Warren e P. Wothers "Organic Chemistry", Oxford University Press, 2001.
- 3- J. March e M.B. Smith "Advanced Organic Chemistry", 5<sup>a</sup> ed. Wiley, 2001.

## MECHANISM OF ORGANIC REACTIONS

### SYLLABUS

1. Experimental determination of the reaction mechanism.
2. Replacement Reactions.
3. Addition reactions to carbon-carbon double bonds.
4. Elimination reactions.
5. Addition reactions to carbon-oxygen double bonds.
6. Reactions of free radicals.
7. Resolution reactions.
8. Oxidation reactions.

### REFERENCES

- 1- F.A. Carey e R.J. Sundberg "Advanced Organic Chemistry", 4<sup>a</sup> ed. Kluwer Academic/Plenum Publishers, 2001.
- 2- J. Clayden, N. Greeves, S. Warren e P. Wothers "Organic Chemistry", Oxford University Press, 2001.
- 3- J. March e M.B. Smith "Advanced Organic Chemistry", 5<sup>a</sup> ed. Wiley, 2001.

## PHYSICAL METHODS IN ORGANIC CHEMISTRY 1

### SYLLABUS

1. Infrared spectrometry.
2. Ultraviolet spectrometry.
3. Mass spectrometry.
4. Proton magnetic resonance spectrometry.
5. Carbon-13 magnetic resonance spectrometry.
6. Joint applications of these techniques.

### REFERENCES

- 1- R.M. Silverstein, F.X. Webster "Spectrometric Identification of Organic Compounds" 7th. Ed John Wiley and Sons, New York, 2005.
- 2- R.M. Silverstein, C.G. Bassler & T.C. Morrill "Spectrometric Identification of Organic Compounds". 5th ed. John Wiley & Sons, 1991.
- 3- P. Crews, J. Rodriguez, M.Jaspars "Organic Structure Analysis" Oxford University Press, New York, 1998.

## PHYSICAL METHODS IN ORGANIC CHEMISTRY 2

### SYLLABUS

1. Discussions on NMR: choice of technique, sample preparation, equipment adjustment, experiment adjustment and data analysis, for the following techniques: 1D: <sup>1</sup>H, <sup>13</sup>C, DEPT135, PENDANT and NOEDIFF; 2D: HHCOSY, HHCOSY-sensitive phase, HHCOSY gradient, phase-sensitive NOESY, HMBC and HMQC.
2. Recent advances in NMR.
3. Mass spectrometry.
4. Recent advances in mass spectrometry.

## REFERENCES

- 1- P. Crews, J. Rodriguez & M. Jaspars "Organic Structure Analysis" Oxford University Press, New York, 1998.
- 2- D.L. Paiva, G.M. Lampman & G.S. Kriz "Introduction to Spectroscopy". 2<sup>nd</sup> ed. Saunders College Publishing, New York, 1996.
- 3- T.D.W. Claridge "High Resolution NMR Techniques in Organic Chemistry". Tetrahedron Organic Chemistry Series, volume 19, Elsevier Science. Amsterdam, 1999.

## LIQUID CROMATOGRAPHY METHODS

### SYLLABUS

1. Fundamental concepts.
2. Separation methods.
3. Separation Optimization.
4. Instrumentation.
5. Gradient Elution.
6. Preliminary Separation.
7. Chiral Separation.
8. Gravity Selective Chromatography.
9. Quantitative and qualitative analysis.
10. Application Examples.
11. Further material: Cass, Q.B. e Degani, A.L.G. Desenvolvimento de métodos por HPLC fundamentos, estratégia e validação, série apontamentos, Editora da UFSCar, 2001.

### REFERENCES

- 1- Lough, W. J. and Wainer, W.; High Performance Liquid Chromatography : Fundamental Principles and Practice; Blackie Academic & Professional, 1995, 1-91p.
- 2- Lindsay, S.; High Performance Liquid Chromatography, 2.ed., John Wiley & Sons, 1992, 1-244p
- 3- Chirality in Natural and applied Science; edited by W. J. Lough and I. W. Wainer, 2002, ISBN 0632-05435-2

## EXPERIMENTAL 1D NUCLEAR MAGNETIC RESSONANCE

### SYLLABUS

1. 1D Specters of: <sup>1</sup>H, <sup>13</sup>C, DEPT135, PENDANT, <sup>19</sup>F and <sup>31</sup>P.
2. Obtainment, processing and printing of specters.

### REFERENCES

- 1- R.J. Abram, J. Fisher e P. Loftus. "Introduction to NMR Spectroscopy. 2<sup>a</sup> ed. John Wiely & Sons, 1995.
- 2- H. Friebolin. "Basic One and Two Dimensional NMR Spectroscopy". VCH, 1993.
- 3- S. Braun, H.O Kalinowski e S. Berger. "150 and More Basic NMR Experiments. A Practical Course". VCH, 2000.

## EXPERIMENTAL 2D NUCLEAR MAGNETIC RESSONANCE

### SYLLABUS

1. 2D Specters of: COSY90, NOESY, HSQC and HMBC.

2. Obtainment, processing and printing of spectra.

## REFERENCES

- 1- R.J. Abram, J. Fisher e P. Loftus. "Introduction to NMR Spectroscopy. 2<sup>a</sup> ed. John Wiley & Sons, 1995.
- 2- H. Friebolin. "Basic One and Two Dimensional NMR Spectroscopy". VCH, 1993.
- 3- S. Braun, H.O Kalinowski e S. Berger. "150 and More Basic NMR Experiments. A Practical Course". VCH, 2000.

## ORGANIC SYNTHESIS METHODOLOGY

### SYLLABUS

1. Single carbon-carbon bond formation.
2. Double carbon-carbon bond formation.
3. Triple carbon-carbon bond formation.
4. Oxidation of organic compounds.
5. Reduction of organic compounds.
6. Transformation of functional groups.
7. Carbon-heteroatom bond formation.
8. Protection and non-protection of functional groups.

### REFERENCE

- 1- F.A. Carey e R.J. Sundberg "Advanced Organic Chemistry" 4<sup>a</sup> ed. Kluwer Academic/Plenum Publishers, 2001.
- 2- J. Clayden e N. Greeves, S. Warren e P. Wothers "Organic Chemistry", Oxford University Press, 2001.
- 3- M.B. Smith. "Organic Synthesis". 2<sup>a</sup> ed. McGraw-Hill, 2002.

## ORGANIC SYNTHESIS

### SYLLABUS

1. Organic Synthesis Methodology.
2. Reaction Selectivity.
3. Organic Synthesis Strategy.
4. Disconnection and Retrosynthetic analysis; sinton.
5. Common atom.
6. Stereocontrol in cyclic, polycyclic and acyclic systems.
7. Natural products synthesis.

### REFERENCES

- 1- M.B. Smith "Organic Synthesis" 2<sup>a</sup> ed. McGraw Hill, 2002.
- 2- K.C. Nicolaou & S.A. Snyder "Classics in Total Synthesis II", Wiley-VCH, 2003.
- 3- J.A. Gewert, J. Gorlitzer, S. Gotze, J. Looft, P. Menningen, T. Nobel H. Schirock e C. Wulff "Organic Synthesis Workbook", Wiley – VCH, 2000.

## ORGANOMETALLIC IN ORGANIC SYNTHESIS

### SYLLABUS

1. Introduction to organometallic chemistry in organic synthesis.
2. Reactions of complexation and discomplexation.

3. Organometallic compounds as protecting and stabilizing groups.
4. Organometallic compounds as electrophiles.
5. Organometallic compounds as nucleophiles.
6. Coupling reactions and cyclization.
7. Isomerization reactions.
8. Oxidation and reduction reactions.
9. Carbonylation reactions.

## REFERENCES

- 1- L.S. Hegedus "Transition Metals in Synthesis of Complex Organic Molecules" University Science Books, 2<sup>a</sup> ed. 1998.
- 2- J. Clayden, N. Greeves, S. Warren & P. Wothers "Organic Chemistry" Oxford University Press, 2001.
- 3- M.B. Smith "Organic Synthesis" 2<sup>a</sup> ed. McGraw Hill, 2002.

## SECONDARY NATURAL PRODUCTS CHEMISTRY

### SYLLABUS

1. Primary and secondary metabolism.
2. Carbohydrates.
3. Shikimic acid and Phenylpropanoid.
4. Flavonoids and oxy-heterocycles.
5. Fatty acids, polyacetylene, acetogenin and postanoids.
6. Terpenes and steroids.
7. Alkaloids.
8. Natural products Spectrometry.

### REFERENCES

- 1- Paul M. Dewick "Medicinal Natural Products: A Biosynthetic Approach" 2<sup>a</sup> ed. John Wiley & Sons, Ltd. 2004.
- 2- J.Mann "Chemical Aspects of Biosynthesis" Oxford University Press, 2002.
- 4- Natural Products Reports: A critical review journal which stimulates progress in all areas of natural products research.

## CHEMICAL ECOLOGY

### SYLLABUS

1. Plant and its biochemistry adaptation to the environment.
2. Biochemistry of pollination.
3. Herbal toxins and their effect on animals.
4. Hormonal interactions between plants and animals.
5. Insects' food preferences.
6. Vertebrates' food preferences, including mankind.
7. Animal pheromones and defensive substances.
8. Biochemical interactions between superior and inferior plants.

### REFERENCES

- 1- Millar, Jocelyn G.; Haynes, Kenneth F. "Methods in chemical ecology". vol.1 e 2 Boston, Kluwer, 1998.

- 2- Howse, Philip E.; Stevens, Ian D.R.; Jones, Owen T. "Insect pheromones and their use in pest management". London: Chapman & Hall, 1998.
- 3- Ferreira, José T.B.; Correa, Arlene G.; Vieira, Paulo C. "Produtos naturais no controle de insetos" São Carlos EdUFSCar, 2001.

## **BIOACTIVY NATURAL PRODUCTS**

### **SYLLABUS**

Natural products and their potential use and mode of action.

Meliaceae Insecticides.

Azadirachtin and other limonoids.

Volatile compounds of plants.

Antimalarials, amebicides.

Antifungals, molluscicides.

Anti-tumor agents.

New properties for old substances.

Discovery and development of drugs.

Enzymes.

### **REFERENCES**

- 1- Barreiro, E.J.; Mansur, C.A. "Química Medicinal: As Bases Moleculares da Ação dos Fármacos" ArtMed Editora Ltda. Porto Alegre, 2001.
- 2- Thomas, Gareth "Fundamentals of Medicinal Chemistry" John Wiley & Sons, Ltd. 2003.
- 3- Patrick, Graham L. "An Introduction to Medicinal Chemistry" Oxford University Press, 2002.

## **TOPICS IN ORGANIC CHEMISTRY**

**Syllabus and References are changeable.**

## **OTHER SUBJECTS**

### **SUPERVISED PRACTICE OF TEACHING CAPACITATION IN CHEMISTRY I**

Elective (6 credits)

#### **SYLLABUS**

Participation of students in mandatory subjects in Chemistry of undergraduate courses at UFSCar. Developed under the supervision of the professor responsible for undergraduate course, activities such as:

- A) Class support.
- B) Preparation and administration of classes.
- C) Preparation of lists of exercises.
- D) Answering questions by students.
- E) Preparation and testing of experiments.
- F) Support in the class activities development.

### **SUPERVISED PRACTICE OF TEACHING CAPACITATION IN CHEMISTRY II**

Elective (6 credits)

#### **SYLLABUS**

Participation of students in mandatory subjects in Chemistry of undergraduate courses at UFSCar. Developed under the supervision of the professor responsible for undergraduate course, activities such as:

- A) Class support.
- B) Preparation and administration of classes.
- C) Preparation of lists of exercises.
- D) Answering questions by students.
- E) Preparation and testing of experiments.
- F) Support in the class activities development .

**Requirements:**

Supervised Practice of Teaching Capacitation in Chemistry 1



## REFORMULATION OF CHEMISTRY TEACHING SUBJECT CURRIULUM

<b>* NEW CURRICULUM OF THE CHEMISTRY TEACHING SUBJECT (VALID FROM 1/2014 ADMISSIONS)</b>	
QUI.401 - PREPARATION OF PROFESSIONAL PROJECT ( <b>Mandatory</b> ) - ( <b>Offered in 1<sup>st</sup> Semester</b> )	New ( <i>NEW SYLLABUS</i> )
Qui.402 Chemistry Foundations A ( <b>Mandatory</b> ) - ( <b>Offered in 2<sup>nd</sup> Semester</b> )	COMBINATION OF FOUNDATIONS 1 AND 2 SUBJECTS (name and syllabus changed)
QUI.403 Chemistry Foundations B ( <b>Mandatory</b> ) - ( <b>Offered in 2<sup>nd</sup> Semester</b> )	Changing of title and syllabus.
QUI.404 Methodological Foundations of Teaching of Chemistry ( <b>Mandatory</b> ) - ( <b>Offered in 1<sup>st</sup> Semester</b> )	No modification
QUI.405 Learning Theories ( <b>Elective</b> )	No modification
QUI.406 Elements and Strategies for the Teaching of Chemistry ( <b>Elective</b> )	No modification
QUI.407 Chemistry Foundations C ( <b>Elective</b> )	New ( <i>NEW SYLLABUS</i> )

### **QUI.401 Preparation of Professional Project** (Mandatory - 10 credits)

PPGQ Accredited Professor

#### **Syllabus:**

1. Identify the research project.
2. Theoretical foundation about the problem.
3. Propose solutions for the problems.
4. Select the appropriate instruments.
6. Discuss implementation viability.
7. Write the project.
8. Evaluation of project, which allows to verify the student's level of knowledge of it: made by an examining commission in a public session specially indicated by CPG and composed of two PhD researchers and the student's supervisor.

#### **References:**

- 1- LAPORTA, Márcia Zorello; ZAMPIERI, Marilim Fogo. Manual para elaboração de trabalhos acadêmicos. São Paulo: Fundação Santo André, 2003. 87 p.
- 2- SEVERINO, Antônio Joaquim. Metodologia do trabalho científico. 22 ed. São Paulo: Cortez, 2002. 355p.
- 3- VOLPATO, Gilson Luiz. Publicação científica. São Paulo : Santana, 2002. 119 p.

### **QUI.402 Chemistry Foundations A** (Mandatory 10 credits)

PPGQ Accredited Professor

#### **Syllabus**

1. Atom: the quantum world.
2. Chemical bonding.
3. Form and structure of molecules.
4. Property of gases.
5. Liquids and Solids.

#### **References**

1. ATKINS, P.; JONES, L. **Princípios de Química**: questionando a vida e o meio ambiente. 5 ed. São Paulo: Bookman, 2012. 1026p.

### **Complementary References**

1. CHANG, R. **Química Geral**: conceitos essenciais. 4 ed. São Paulo: McGraw-Hill, 2006. 778p.
2. BROWN, T. L.; LE MAY, H. E.; BURSTEN, B. E. **Química**: a ciência central. 9 ed. Pearson/Prentice Hall, 2005. 972p.

### **QUI.403 Chemistry Foundations B** (Mandatory - 10 credits)

PPGQ Accredited Professor

#### **Syllabus**

1. Stoichiometry: balancing and calculations.
2. Thermodynamics: the first law.
3. Chemical Balances.
4. Acids and bases.
5. Balance in Water.
6. Electrochemistry.
7. Chemical Kinetics.

#### **References**

1. ATKINS, P.; JONES, L. **Princípios de Química**: questionando a vida e o meio ambiente. 5 ed. São Paulo: Bookman, 2012. 1026p.

### **Complementary References**

1. CHANG, R. **Química Geral**: conceitos essenciais. 4 ed. São Paulo: McGraw-Hill, 2006. 778p.
2. BROWN, T. L.; LE MAY, H. E.; BURSTEN, B. E. **Química**: a ciência central. 9 ed. Pearson/Prentice Hall, 2005. 972p.

### **QUI.404 Methodological Foundations of Teaching of Chemistry** (Mandatory - 10 credits)

PPGQ Accredited Professor

#### **Syllabus**

1. Part One: Overview of Chemistry teaching and main research tendencies.
2. Part Two: Specific teaching-learning process in Chemistry.

Language and meaning:

- Learning of concepts and problem solving;
- Chemistry knowledge fundamental aspects;
- Approaches to theoretical and experimental teaching of Chemistry;
- Content and evaluation.

3. Part Three: Educational projects in Chemistry:

- Theoretical frame;
- Research problems;
- Collection procedure;
- Analysis;
- Research report.

#### **References**

1. CARVALHO A.M.P. (org.). Ensino de ciências: unindo a pesquisa e a prática. Pioneira Thomson Learning, São Paulo, 2004.
2. SANTOS, W. L. P. e SCHNETZLER, R. P. Educação em química: compromisso com a cidadania. Ijuí : Editora da Ijuí, 2003.
3. ALVES-MAZZOTTI, ALDA JUDITH & GEWANDSZNAJDER, FERNANDO. O método das ciências naturais e sociais: pesquisa quantitativa e qualitativa. São Paulo: Pioneira Thonsom, 2002.

### **QUI.405 Learning Theories** (Elective - 4 credits)

PPGQ Accredited Professor

#### **Syllabus**

The following theories are considered in cognitive and affective aspect area.

General and historical introduction.

Piaget's cognitive development theory.

Vygotsky's theory and social interaction.

Ausubel's significant learning theory.

Vovak's educational theory and Gowin's teaching-learning model.

Information processing theory.

#### **References**

1- COLL, CESAR; PALACIOS, JESUS E MARCHESI, ALVARO. Desenvolvimento Psicológico e educação: psicologia da educação. Porto Alegre - Artes Médicas, 2001.

2- CÉSAR COLL SALVADOR Psicologia do ensino. - Porto Alegre – ARTMED, 2000.

3-MOREIRA M.A. A teoria da aprendizagem significativa e sua implementação em sala de aula. Brasília - Editora Unb, 2006.

### **QUI.406 - Elements and Strategies for the Teaching of Chemistry** (Elective 4 credits)

PPGQ Accredited Professor

#### **Syllabus**

1. Relations between concepts on Science nature and teaching practice.

2. Student's alternative conceptions related to Chemistry contents.

3. Strategies for the Teaching of Chemistry.

4. Innovate approaches to the teaching of Chemistry, STS, islands of interdisciplinary rationality, etc.

5. Experimentation role to the teaching of Chemistry.

6. Chemistry history role to the teaching of Chemistry.

#### **References**

1. MALDANER, OTÁVIO A. A Formação Inicial e Continuada de Professores de Química. Ed. UNIJUÍ, Ijuí, 2000.

2. MACHADO, ANDRÉA H. Aula de Química: Discurso e Conhecimento. Ed. UNIJUÍ, Ijuí, 1999.

3. Articles from the journals: - Química Nova (Revista da Sociedade Brasileira de Química) - Journal of Chemical Education (Revista da Divisão de Ensino de Química da American Chemical Society).

### **QUI.407 Chemistry Foundations C** (Elective - 10 credits)

PPGQ Accredited Professor

#### **Syllabus**

1. Thermodynamics: second and third laws.

2. Physical balances.

3. Inorganic materials.

4. Organic Chemistry: polymers and biological compounds.

5. Environmental Chemistry.

## 6. Nuclear Chemistry.

### References

1. ATKINS, P.; JONES, L. **Princípios de Química**: questionando a vida e o meio ambiente. 5 ed. São Paulo: Bookman, 2012. 1026p.

### Complementary References

1. CHANG, R. **Química Geral**: conceitos essenciais. 4 ed. São Paulo: McGraw-Hill, 2006. 778p.
2. BROWN, T. L.; LE MAY, H. E.; BURSTEN, B. E. **Química**: a ciência central. 9 ed. Pearson/Prentice Hall, 2005. 972p.

## PROFESSIONAL MASTER'S DEGREE – TECHNOLOGICAL CHEMISTRY AREA

Mandatory

QUI.601 [Preparation of Professional Project](#)

QUI.602 [Advanced Chemistry](#)

Elective

[Topics in Technological Chemistry – Introduction to Macromolecular Architecture](#)

### Preparation of Professional Project

PPGQ Accredited Professor

#### Syllabus

1. Dimension specific research problems, non-conventional academic development and innovation of a company.
2. Theoretical foundations about the problem theme.
3. Propose solutions to specific research problems, non-conventional academic development and innovation of a company.
4. Select requested instrumental techniques.
5. Quality control.
6. Implementation viability of the Project, granting a better return on investment, aiming productive and qualitative gains.
7. Writing the project.
8. Evaluation of the project, which allows to solve the company problem: made by an examining commission in a public session specially indicated by CPG and composed of two PhD researchers and the student's supervisor. One of the two PhD researchers may be from the company where the student develops the project, whereas requested to CPG.

#### Refences

- 1- LAPORTA, Márcia Zorello; ZAMPIERI, Marilim Fogo. Manual para elaboração de trabalhos acadêmicos. São Paulo: Fundação Santo André, 2003. 87 p.
- 2- SEVERINO, Antônio Joaquim. Metodologia do trabalho científico. 22 ed. São Paulo: Cortez, 2002. 355p.
- 3- VOLPATO, Gilson Luiz. Publicação científica. São Paulo : Santana, 2002. 119 p.

### Advanced Chemistry

PPGQ Accredited Professor

#### Syllabus

1. This subject is composed by 4 sequential modules that present in each one the traditional subareas of Chemistry:

Module 1: Physic-chemical

1. Chemical Thermodynamics :first and second laws and free energy (2 classes).
2. Chemical kinetics: reaction speed, activation energy, collision and activated complex theories (1 class).
3. Introduction to quantum chemistry: Bohr atom, quantum model and Schrödinger equation (1 class).

Module 2: Analytical Chemistry

1. Acid-base balance.
2. Solubility balance.
3. Complexation balance.
4. Oxy-reduction Balance.

Module 3: Inorganic Chemistry

1. Chemical bonds: ionic and covalent compounds.
2. Matter structure and reactivity.
3. Inorganic materials.

Module 4: Organic Chemistry

1. Stereochemistry / Conformational analysis.

2. Organic acids and bases: Pearson's concept.
3. Chemistry of enolates.
4. A view of catalysis in Organic Chemistry.

2. Each module shall run for one month and shall be independently evaluated by the professor.

#### References

1. P. Atkins e L. Jones, Princípios de Química, Ed. Bookman, 2005.
2. P. Atkins, Physical Chemistry, Ed. Oxford University Press, 1998.
3. A. J. Bard, Chemical Equilibrium, Harper & Row, 1966.
4. R. Kellner, J. M. Mermet, M. Otto, M. Valcarcel e H. M. Widmer, Analytical Chemistry: A modern approach to analytical science, Wiley-VCH, 2004.
5. J. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry, Pearson, 1993.
6. N. Hall, The new chemistry, Cambridge University Press, 2000.
7. Strategic Applications of Named Reactions in Organic Synthesis - László Kurti and Barbara Czákó, 1 edition - 2005, Elsevier Academic Press.
8. Jonathan Clayden, Nick Greeves, Stuart Warren and Peter Wothers, Organic Chemistry, Oxford University Press, 1ª edição, 2001.
9. Ácidos e Bases em Química Orgânica, P. Coelho, V. Ferreira, P. Esteves, M. Vasconcellos, Bookman, SBQ, 2005

---

### Topics in Technological Chemistry – Introduction to Macromolecular Architecture

**Prof. Dr. Mitsukimi Tsunoda**

#### Syllabus

- 1- Generalities about macromolecules.
- 2- Types of macromolecular systems.
- 3- Preparations methods.
- 4- Types of interaction involving macromolecular species.
- 5- Applications.

#### References

- 1- P. Ball "Designing the molecular world – chemistry at the frontier". Princeton University Press, Princeton, 1994.
- 2- P.D. Beer, P.A. Gale, D.K. Smith "Supramolecular Chemistry" Oxford University Press. Oxford, 1999.
- 3- O. Costisor, W. Linert "Metal Mediated Template Synthesis of Ligands", World Scientific, New Jersey, 2004.