UNIVERSIDADE ESTADUAL DE CAMPINAS
INSTITUTO DE QUÍMICA

PROGRAMS AND BIBLIOGRAPHY

Subject	
Code	**Name**
QF531	Physical Chemistry II

Vector
OF:S-5 T:004 P:000 L:000 O:000 D:000 HS:004 SL:004 C:004 AV:N EX:S FM:75%

Pre requirement	QF431/QF335

Summary

The kinetic theory of gases: barometric equation, the Maxwell-Boltzmann velocity distribution, intermolecular potential. Chemical kinetics: rate equations, homogeneous and heterogeneous catalysis; fast reactions, notions on molecular dynamics. Electrochemistry: solution conductivity, Ostwald dilution law, ionic equilibrium, thermodynamic properties, activity coefficients, Debye-Hückel theory, batteries and electrochemical reactions, passivation and corrosion.

Program

I. Chemical Equilibrium
- Reactions in the gaseous state; reaction progress.
- Reactions in condensed phase.
- Solutions of electrolytes. Activity.

II. Electrochemistry
- Reactivity of metals.
- Batteries, standard EMF, Nerst equation, relation between EMF, deltaG, deltaH, deltaS, electrode potential and applications.
- Theories of Arrhenius and Debye-Hückel; Debye-Hückel limiting law; ionic conductivity.

III. Chemical kinetics
- Reaction rate. Average and instantaneous reaction rates. Empirical kinetic laws. The role of temperature.
- Interal equations, half-life.
- Mechanisms: elementary reactions, reversible reactions, irreversible reactions, and consecutive reactions.
- Detailed balance, steady state approximation and other approximations.
- Homogeneous and heterogeneous catalysis.
- Polymerization, radical, photochemical and enzymatic (Michaelis-Menten) reactions.

IV. The kinetic theory of gases
- Kinetic energy and temperature.
- The Maxwell-Boltzmann equation of velocities. Brownian motion, diffusion.
- Collision frequency, mean free path, collision cross-section.
- Relation between reaction rates, collision frequency and collision energy.
- Notions on activated complex theory.

Bibliography

1. *Molecular Thermodynamics*, D. A. McQuarrie e J. D. Simon. Scientific Books (Grande parte do material pode ser encontrada também no texto "*Physical Chemistry: A Molecular Approach*" dos mesmos autores.
2. *Physical Chemistry* (2a ed.), R. A. Alberty & R. J. Silbey.
3. *Physical Chemistry*, I. Levine.
4. *Physical Chemistry*, P. W. Atkins.
5. *Termodinâmica Química*, Aécio Pereira chagas, Ed. Unicamp, 1999.

Evaluation criteria

Critérios de avaliação definidos pelo Professor, com base no disposto na Seção I – Normas Gerais, Capítulo V – Da Avaliação do Aluno na Disciplina, do Regimento Geral de Graduação. Frequência: 75 % (* O abono de faltas será considerado dentro do previsto no capítulo VI, seção X, artigo 72 do Regimento Geral de Graduação)