Code: **QF531**

Name: **Físico-Química II**

Name in English: **Physical Chemistry II**

Name in Spanish: **Físicoquímica II**

Subject type: **Weekly**

Approval Type: **Grade and Attendance**

Characteristic: **Regular**

Frequency: **75%**

Period Type / Offering period: **Semester / All periods**

Requires Final Exam: **Yes**

Vectors

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

Occurrence on curriculum: **05, 13, 50, 56**

Pre requirement: **QF431 ou QF335 ou QF331**

Summary: **Kinetic theory of gases: barometric equation, Maxwell-Boltzmann Law for velocity distribution; intermolecular potential. Chemical kinetics: rate equations; homogeneous and heterogeneous catalysis; fast reactions, molecular dynamics concepts. Electrochemistry: conductivity of solutions, Ostwald's Law; ionic equilibrium; thermodynamic properties; activity coefficients; Debye-Hückel theory; cells and electrochemical reactions; passivation and corrosion.**

Program:

I. Chemical Equilibrium

- Gas-phase reactions; reaction progress.
- Condensed phase reactions.
- Electrolyte solutions. Activities.

II. Electrochemistry - Reactivity of metals

- Cells, standard EMF, Nernst Equation, relationship between EMFs, deltaG, deltaH, and deltaS, electrode potential and applications.
- Arrhenius and Debye-Hückel theory; D-H limiting law; ionic conductivity.

III. Chemical Kinetics

- Reaction rate, average and instantaneous velocities; empirical kinetic laws, temperature effect.
- Integrated equations, half-life.
- Mechanisms: Elementary, reversible, irreversible, and consecutive reactions; equilibrium detail ratio; steady-state and other approximations.
- Homogeneous and heterogeneous catalysis.
- Polymerization reactions, radical, photochemical, enzymatic (Michaelis-Menten).

IV. Kinetic Theory of Gases

- Kinetic energy and temperature.
- Velocity distribution (Maxwell-Boltzmann), Brownian motion, diffusion.
- Collision frequency, mean free path, cross-section.
- Relationship between reaction rate, collision rates, and collision energy.

- Notions about the activated complex theory.

Basic Bibliography

1) McQUARRIE, D. A.; SIMON, J. D. **Physical Chemistry: A Molecular Approach.** 1. Ed. University Science Books, 1997. 1360 p
2) LEVINE I. N. **Physical Chemistry.** 6 Ed. McGraw-Hill, 2008. 1008 p
3) ATKINS, P W.; PAULA, J.; **Physical Chemistry: Thermodynamics, Structure and Change.** 10 Ed. Oxford University Press, 2018. 1060 p

Supplementary Bibliography

1) CHAGAS, A. P. **Termodinâmica Química.** 1 Ed. Editora da UNICAMP, 2019. 409 p
2) ATKINS, P.; JONES, L.; LAVERMAN, L. **Princípios de química: questionando a vida moderna e o meio ambiente.** 7. Ed. Porto Alegre: Bookman, 2018. 830 p
3) SIMON, J.; MCQUARRIE, D. A. **Molecular Thermodynamics**. 1 Ed. University Science Books, 1999. 672 p
4) MCQUARRIE, D. A. **Statistical Mechanics**. 1 Ed. University Science Books, 2000. 641 p
5) KLIPPENSTEIN, S. J.; PANDE V. S.; TRUHLAR, D. G. **Chemical Kinetics and Mechanisms of Complex Systems: A perspective on recent theoretical advances.** J. Am. Chem. Soc. 2014, 136, 2, 528–54