

COURSE SYLLABUS

1. Identification

Code and title: QUP 303 – Advanced Physical Chemistry

Professor: Paulo Augusto Netz, Maximiliano Segala and Paulo Fernando Bruno Gonçalves

Level: Master and Doctorate

Credit hours: 3

Revised: August_2021

2. Summary

Classical thermodynamics of ideal and non-ideal systems. Alternative formulations of the second principle. Non-equilibrium thermodynamics: fundamentals, linear and non-linear regime and dissipative structures

3. Objective

Introduce the student to physical-chemical concepts of real systems and their temporal evolution, with a thermodynamic approach

4. Contents

- Alternative approaches to classical thermodynamics of ideal and non-ideal systems
- Second Principle Approach according to Caratheodory, Boltzmann and Prigogine
- Calculation of variations for thermodynamic extremes
- Thermodynamic stability criteria
- Non-equilibrium thermodynamics: entropy production, Onsager relations, transport, dissipation
- Non-equilibrium thermodynamics: steady state, non-linear systems, instabilities and oscillations

5. Assessment

List of exercises, presentation and discussion of scientific articles, theoretical tests and/or directed works. The student, who obtains a final grade of A, B or C, awarded as per the list below, will be considered approved:

A: grade equal to or above 9.0

B: grade equal to or above 7.5 and below 9.0

C: grade equal to or above 5.0 and below 7.5

D: grade below 5

FF: lack of frequency

6. Methodology

Lectures, exercises lists, seminars and examinations.

7. Bibliography

- I. Prigogine e D. Kondepudi, Termodinâmica: dos motores térmicos às estruturas dissipativas, Instituto Piaget, 1999.



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- S. M. Blinder, Advanced Physical Chemistry, London, Macmillan, 1969.
- D. A. McQuarrie e J. T. Simon, Physical Chemistry: A Molecular Approach, University Science Books, 1997.
- S. R. Degroot and P. Mazur, Non-Equilibrium Thermodynamics, North-Holland, 1976.
- H. J. Kreuzer, Non-Equilibrium Thermodynamics and its Statistical Foundations, Clarendon Press, 1983.
- B. H. Lavenda, Thermodynamics of Irreversible Processes, New York, Dover, 1993.