

208001 – ADVANCED PHYSICAL-CHEMISTRY I

CREDITS: 04 (four) – 60 hours/class

CONTENT:

Concepts of work and heat. The First Law of Thermodynamics and its implications and applications. Second and Third Laws of Thermodynamics (the concept of entropy). Definition of free energy. Chemical balance. Thermodynamics of solutions. General aspects of kinetic chemistry.

SYLLABUS:

1. Gaseous systems, deviations of ideality, Van der Waals fluid and models based on cubic equations.
2. Work, heat and energy. Reversible, quasi-static processes and reversibility.
3. Thermodynamic potentials at the limit of reversibility, Maxwell relations and thermodynamic state equations.
4. Interaction between particles, theoretical interpretation about the second coefficient of the virial series and the L-J potential well.
5. Theory of chemical reactions and the statistical mechanics fundamentals of the absolute velocity's theory (activated complex) for the simple bimolecular process in gas phase.
6. The relationship between thermodynamics and kinetics according to Eyring's interpretation.

BIBLIOGRAPHY:

1. ATKINS Peter; PAULA, Júlio de. Físico-Química. 8.ed. LTC, 2008.
2. CASTELLAN, G. Fundamentos de Físico-Química. LTC, 1989.
3. McQUARRIE, Donald A.; SIMON, John D. Physical Chemistry: a molecular approach. University Science Books, 1997.