212031 – STATISTICAL THERMODYNAMICS

CREDITS: 04 (four) – 60 hours/class

CONTENT:

Introduction to Probability and Statistics. Boltzmann distribution and partition function. Partition function and thermodynamic properties.

SYLLABUS:

1. Kinetic theory of gases.
2. Gaussian distribution and energy distribution curves.
3. Entropy as a statistical concept.
4. Definition of canonical fitting and partition function.
5. Electronic, Vibrational and Rotational Partition Functions.
6. Definitions of internal energy, entropy and heat capacity from the partition function.
7. Statistical thermodynamics applied to the analysis of vibrational spectra.

BIBLIOGRAPHY:

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