UNIVERSIDADE ESTADUAL DE CAMPINAS
INSTITUTO DE QUÍMICA

PROGRAMS AND BIBLIOGRAPHY

Subject	
Code	**Name**
QF637	Introduction to Spectroscopy and Statistical Thermodynamics

Vector
OF:S-1 T:004 P:000 L:000 O:000 D:000 HS:004 SL:004 C:004 AV:N EX:S FM:75%

Pre requirement	QF536 *F 428

Summary

Molecular spectroscopy. Electron paramagnetic resonance (EPR) spectroscopy and nuclear magnetic resonance (NMR) spectroscopy. Lasers. Photochemistry. Ensembles and postulates. Partition functions and thermodynamics. Systems of independent particles: distinguishable and indistinguishable. Applications.

Program

I. Introduction to Spectroscopy

1. Review of Quantum Mechanics: postulates and the Schrödinger equation. Quantum states of the particle in a box, hydrogen atom, harmonic and anharmonic oscillator and rigid rotor. Orbital and magnetic angular momenta. Spins.
2. Time-dependent perturbation theory (transition probability; transition moment).
3. The electromagnetic spectrum and matter-radiation interaction.
4. Rotational spectroscopy.
5. Rovibrational spectroscopy.(infrared and Raman).
6. Electronic spectroscopy (vibronic transitions).
7. Lasers.
8. Nuclear and electronic magnetic resonance.
9. Photochemistry and photophysics.
10. Stationary spectra and time-resolved spectroscopy.

II. Introduction to Statistical Thermodynamics

1. Review of thermodynamics: 1st, 2nd, and 3rd laws.
2. Macrostates, microstates and configurations.
3. Counting and entropy: Boltzmann distribution.
4. Partition functions and ensembles.
5. Systems of independent particles.
6. Ideal gases; polyatomic ideal gases.
7. Chemical equilibrium: a detailed microscopic view.

Bibliography

1- Physical Chemistry: A Molecular Approach", D. A. McQuarrie e J. D. Simon.
2- Molecular Thermodynamics, D. A. McQuarrie e J. D. Simon. Scientific Books.
3- Statistical Mechanics, D. A. McQuarrie.
4- Physical Chemistry, R. A. Alberty & R. J. Silbey
5- Physical Chemistry, I. Levine.

Evaluation criteria

For grading policy, see: Regimento Geral de Graduação, Seção I – Normas Gerais, Capítulo V – Da Avaliação do Aluno na Disciplina. Students are required to attend 75 % of the lectures. For further details, see: Regimento Geral de Graduação, capítulo VI, seção X, artigo 72.