212002 – MOLECULAR SPECTROSCOPY

CREDITS: 04 (four) – 60 hours/class

CONTENT:

Introduction to vibrational spectroscopy: harmonic and anharmonic oscillator, classical and quantic energies, vibrational models in infrared and Raman; Rotational and ro-vibrational spectroscopy; Introduction to group theory; Solving the molecular vibration: force field and normal coordinate analysis for simple chemical systems; Raman effect: quantum model for light scattering; special effects: resonance Raman and surface-enhanced Raman scattering.

SYLLABUS:

1. Introduction to vibrational spectroscopy: Newton's laws, Lagrange equations, quantum model for the vibrational frequency.
2. Harmonic oscillator and anharmonic oscillator approaches: potential energy for the ball-springsystem and application to chemical models.
3. Introduction to infrared spectroscopy: equations and main applications.
4. Introduction to rotational spectroscopy: classical and quantum models and applications.
5. Normal coordinate analysis: introduction and application of group theory and point groups.
6. Normal coordinate analysis: the molecular vibration problem in the normal coordinate analysis; the secular equation.
7. Experimental: normal coordinate calculation for simple chemical systems, involving few atoms.
8. Special Raman effects: resonance Raman.
9. Special Raman effects: surface-enhanced Raman scattering (SERS).

BIBLIOGRAPHY:

1. McHALE, Jeanne L. Molecular Spectroscopy. Prentice-Hall, USA, 1999.
2. SALA, Oswaldo. Fundamentos da Espectroscopia RAMAN e no Infravermelho. 2ndEd. Editora da UNESP, Brasil, 2008.
3. HARRIS, Daniel C.; BERTOLUCCI, Michael D. Symmetry and spectroscopy: an introduction to vibrational and electronic spectroscopy. Dover Publications, USA, 1999.
4. COLTHUP, Norman B.; DALY, Lawrence H.; WIBERLEY, Stephen E. Introduction to Infrared and RAMAN Spectroscopy. 3.ed. Academic Press, USA, 1990.