Code: **QG664**

Name: **Espectroscopia Molecular**

Name in English: **Molecular Spectrocospy**

Name in Spanish: **Espectroscopia Molecular**

Subject type: **Weekly**

Approval Type: **Grade and Frequency**

Characteristic: **Regular**

Frequency: **75%**

Period Type / Offering period: **Semestral / 2nd Period – even periods**

Requires Final Exam: **Yes**

Vectors

T	L	P	O	PE	OE	SL	WEEKS	CREDITS
2	**2**	**-**	**0**	**-**	**-**	**4**	**15**	**4**

Occurrence on curriculum: **5**

Pre requirement: **QF536 + *QI145 ou QF536 + *QI146**

Program: Group theory. Rotational, rotational-vibrational and electronic spectroscopies. Selected experiments.

Program:

1) Radiation-matter interaction: classical descriptions of atoms/molecules and radiation

Concepts: frequency; radiation intensity; classical damped harmonic oscillator (polarizability), absorption and dispersion; bandwidths; Lambert-Beer law; Experimental measurements: experimental apparatus for light absorption (transmission/absorption).

Connection to experiments: (i) classical concept of resonance in light-matter interaction: the molar absorptivity measurement for different molecules (for instance rhodamine) and experimental measurement of molecular polarizability. Relationship between molar absorptivity and absorption intensity; (ii) electric dipole measurement of polar molecules in solution.

2) Radiation-matter interaction: quantum descriptions of atoms/molecules and classical description of radiation

Concepts: Einstein coefficients (two level systems); relationship among Einstein coefficients; transition probabilities; transition intensity and molar absorptivity; light-matter interaction Hamiltonian; time-dependent perturbation theory; transition dipole moment; Fermi golden rule.

Connection to experiments: (i) atomic absorption/emission spectroscopy and comparison with hydrogen atom model; Note: various experiments/data acquisition can be performed in the same day.

3) Vibrational, rotational e rotational-vibrational spectroscopy of diatomic molecules.

Concepts:

(I) Vibrational: harmonic oscillator; potential energy curve; symmetry of wavefunctions; selection rules; overtones; infrared absorption and Raman activities.

(II) Rotational: rigid rotor; angular momentum; Boltzmann distribution; selection rules and absorption and Raman rotational spectroscopies.

(III) Rotational-vibrational: fine rotational structure in vibrational transitions.

Connection to experiments:

(I) Infrared absorption of HCl (liquid); Raman spectroscopy of I_2.

(II) Rotational-vibrational spectrum of HCl (gas)

4) Vibrational spectroscopy of polyatomic molecules

Concepts: Group theory; vibration normal modes; characteristic frequencies; combination and overtone bands. Infrared and Raman activities.
Connection to experiments: (i) vibrational spectrum of CO_2 and determination of normal modes from first principles and group theory; (ii) water vibrational spectrum: solid, liquid and gas; (iii) vibrational spectra: polyatomic molecules and group theory; Note: various experiments/data acquisition can be performed in the same day.

5) Electronic spectroscopy
Concepts: hydrogen atom; diatomic and polyatomic molecules; selection rules; vibronic structure; emission; molecular orbital theory; ligand field theory; group theory; anharmonic potential energy curves in ground and excited states.
Experiments in electronic spectroscopy: (i) diatomic molecules: iodine as model for absorption and fluorescence; (ii) polyatomic molecules: group theory and molecular orbital theory; (iii) polyatomic molecules: group theory and ligand field theory; (iv) solid, liquid and gas. Note: various experiments/data acquisition can be performed in the same day.

Basic Bibliography

1) SALA, O. **Fundamentos da Espectroscopia Raman e no Infravermelho.** 2a ed. São Paulo: Editora UNESP, 2008. 276 p.
2) NAKAMOTO, K. **Infrared and Raman spectra of Inorganic and Coordination Compounds – Part A and Part B.** 6th ed. New York: John Wiley, 2009.
3) ATKINS, P., DE PAULA, J. **Physical Chemistry.** 9th ed. New York: W.H. Freeman and Company, 2010, 1010 p.
4) MCQUARRIE, D.A., SIMON, J.D. **Physical Chemistry: a Molecular Approach.** University Science Books, 1997. 1360 p.

Supplementary Bibliography

1) MIESSLER, G. L., TARR, D. A. **Inorganic Chemistry.** 4th ed., Harlow: Pearson, 2011. 1213 p.
2) KETTLE, S. F. A. **Symmetry and Structure: (Readable Group Theory for Chemists).** 2nd ed. Chichester: John Wiley, 1995. 416 p.
3) LEVER. A. B. P. **Inorganic Electronic Spectroscopy.** 2nd ed. Amsterdam: Elsevier, 1984. 863 p.
4) HARRIS, D.C., BERTOLUCCI, M.D. **Symmetry and Spectroscopy.** 1a ed. revisada. Dover Publications, 1989. 576 p.
5) SKOOG, D.A., HOLLER, F.J., CROUCH, S.R. **Principles of Instrumental Analysis.** 7th ed. Cengage Learning, 2017. 992 p.