Code: **QF530**

Name: **Introdução à Química Quântica e Espectroscopia Molecular**

Name in English: **Introduction to Quantum Chemistry and Molecular Spectroscopy**

Name in Spanish: **Introducción a la Química Cuántica y Espectroscopia Molecular**

Subject type: **Weekly**

Approval Type: **Grade and Attendance**

Characteristic: **Regular**

Frequency: **75%**

Period Type / Offering period: **Semester / All periods**

Requires Final Exam: **Sim**

Vectors

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

Occurrence on curriculum: **05, 50, 56**

Pre requirement: ***MA311**

Summary: **Notions of Spectroscopy and Postulates of quantum mechanics. Particle in the box and electronic structure. Rigid rotor and rotational spectroscopy of diatomic molecules. Harmonic oscillator and vibrational spectroscopy of diatomic molecules. Roto-vibrational spectroscopy of diatomic molecules. Electronic structure, ground and excited states. Photochemistry and photophysics.**

Programa:

1. Notions of Spectroscopy and Postulates of quantum mechanics. Interaction of radiation with matter: absorption, emission, scattering, and diffraction. Einstein coefficients, notions of laser, transition moment, and selection rules, blackbody radiation and Broglie waves. Postulates of quantum mechanics: well-behaved wave functions, operators, and property calculation, time-dependent and time-independent Schrödinger equation. Applications in the particle in the box model and relationship with electronic spectroscopy.
2. Roto-Vibrational Spectroscopy. Rotational spectroscopy in the microwave region and notions of instrumentation. Rigid rotor model, spectra of diatomic molecules, and selection rules. Infrared spectroscopy and notions of instrumentation. Harmonic and anharmonic oscillator model. Analysis of roto-vibrational spectra of diatomic molecules and selection rules. Raman spectroscopy and selection rules.
3. Electronic Structure. UV-vis spectroscopy instrumentation. The hydrogen atom. Electronic emission and absorption spectra and selection rules. Notion about Stark and Zeeman effect. Hamiltonian operator for multi-electronic systems. Spin, Pauli exclusion principle, and Slater determinants. Molecules and Born-Oppenheimer approximation. Notion about the Hartree-Fock method. Variational principle and linear combination of atomic orbitals. Application in molecules. Hückel method and pi systems. UV-visible absorption and emission spectroscopy. Notions of photochemistry and photophysics.

Basic Bibliography

1) MCQUARRIE, D. A.; SIMON, J. D. **Physical Chemistry: A Molecular Approach.** 1. Ed. Sausalito: University Science Books, 1997. 1360 p

2) BARROW, G. M. **Introduction to Molecular Spectroscopy**. 1. Ed. Tóquio: McGraw-Hill. 1962. 318 p

3) LEVINE, I. **Físico-Química**. 6. Ed. Rio de Janeiro: Livros Técnicos e Científicos, 2012. 2v 1008p

Supplementary Bibliography

1) SALA O., **Fundamentos da Espectroscopia Raman e no Infravermelho.** 2. Ed. São Paulo: Editora Unesp, 2011. 280 p
2) PAULING, L.; WILSON, E. B. **Introduction to Quantum Mechanics with Applications to Chemistry**. 1. Ed. New York: McGraw-Hill, 1935. 468 p
3) HERZBERG, G. **Molecular spectra and molecular structure Volume I - Spectra of Diatomic Molecules.** 2. Ed. Malabar: Krieger Publishing. 1989. 660p
4) PAVIA, D.; LAMPMAN, G.; KRIZ, G.; VYVYAN, J. **Introdução à espectroscopia**. 2. Ed. São Paulo: Cengage Learning. 2015. 733p
5) ATKINS, P. W.; DE PAULA, J. **Físico-Química: fundamentos.** 9. Ed. Rio de Janeiro: Livros Técnicos e Científicos. 2012. 2v. 948p