Code: **QI445**

Nome: **Introdução à Espectroscopia Vibracional**

Nome em Inglês: **Introduction to Vibrational Spectroscopy**

Nome em Espanhol: **Introducción a la Espectroscopia Vibracional**

Subject type: **Semesterly**

Approval type: **Grade and Attendance**

Characteristic: **Regular**

Frequency: **75%**

Period Type / Offering period: **Semesterly / second semester**

Requires Final Exam: **Sim**

Vetores

T	L	P	O	PE	OE	SL	SEMANAS	CRÉDITO
2	**-**	**-**	**-**	**-**	**-**	**2**	**15**	**2**

Occurrence on curriculum: **63**

Pre requirement: **QI245 ou QI246**

Summary: **Fundamental on vibrational spectroscopy and interpretation of spectra**

Fundamentals (electromagnetic radiation - regions / range of frequencies / techniques; Classical and Quantum Theories of radiation interpretation);
- Transitions: electronic / vibrational / rotational, associating them with spectral regions and analysis techniques;
- Energy levels of diatomic molecules;
- Vibrational spectrum - Selection rules for IR and Raman;
- Classic model of energy absorption for vibration;
- Quantum model of energy absorption for vibration;
- fundamental or normal modes of vibration;
- Types of molecular vibrations;
- Diatomic molecules: normal modes of vibration, character table, analysis of vibration frequencies, correlation with bond strength;
- Molecules X3 and YXY, linear and angular (analysis of vibration frequencies for XH2 molecules and isotopic);
- Molecules XY3;
- Molecules XY4, ZXY3; and Z2XY2: Use of the Correlation Tables;
- Group frequencies and band assignment;
- IR spectrum ofcomplex molecules using group frequencies: coordination complexes, coordination effect, nature of the central atom;
- Complexes with NH3; nitro-nitrite; sulfates; carbonyls;
- Hydrogen bonds and molecular associations;
- ATR and DRIFTS,
- Visit to the equipment;
- Sampling techniques;
- Preparation of samples versus spectrum quality, most usual sampling (concentration effect, optical path, sample dispersion).

Bibliography

1) NAKAMOTO, K. **Infrared and Raman spectra of inorganic and coordination compounds**, 4th Ed. New York, 1986.
2) BELLAMY, L.J. **"The infrared spectra of complexes",** 2nd Ed., London, Meuthuen, 1966.
3) BELLAMY, L.J. **"Advances in infrared group frequencies",** 2nd Ed., London, Meuthuen, 1968.

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.