UNIVERSIDADE ESTADUAL DE CAMPINAS
INSTITUTO DE QUÍMICA

PROGRAM AND BIBLIOGRAPHY

Subject	
Code	**Nome**
QG664	Molecular Spectroscopy

Vector
OF:S-2 T:002 P:000 L:002 O:000 D:000 HS:004 SL:004 C:004 AV:N EX:S FM:75%

Pre Requirement	QF536 QI145

Summary

Group Theory. Rotational, rotational-vibrational and electronic spectroscopy. Selected experiments.

Program

1) Interaction of radiation with matter: classical "atom", classical radiation
Concepts: frequency; intensity of radiation; classical harmonic oscillator, forced and damped (polarizability), absorption and dispersion; line widths; Law of Lambert-Beer;
Experimental measurements: Experimental apparatus for light absorption measurement (transmission / absorption);
Relation of experiments: (i) the classical concept of resonance in light absorption: measure of molar absorptivity for different molecules (eg rhodamine) and experimental measure of molecular polarizability. Relationship between molar absorptivity and absorption intensity; (ii) measurement of the electric dipole moment of polar molecules in solution.

2) Interaction of radiation with matter: quantum "atom", classical radiation
Concepts: Einstein coefficients (two-level systems); relationship between Einstein coefficients, transition probability, transition intensity and molar absorptivity; Hamiltonian interaction of matter / radiation; theory of time-dependent perturbation; transition dipole moment; Fermi's rule of thumb;
Relation of experiments: (i) atomic absorption / emission spectrometry and comparison with hydrogen atom model; Note: Multiple experiments / data collection can be performed in a single day.

3) Vibrational, rotational and roto-vibrational spectroscopy of diatomic molecules.
Concepts:
(I) Vibrational: harmonic oscillator, potential energy curve, symmetry of wave functions; selection rules; Overtones; Activity in IR and Raman.
(II) Rotational: rigid rotor; angular momentum; Boltzmann distribution; selection rule and rotational absorption and Raman scattering spectroscopy;
(III) Roto-vibrational: Fine rotational structure.
Relation with experiments:
(I) Infrared absorption spectroscopy of HCl (liquid). Raman spectroscopy of I_2.
(II) and (III) Rotovibrational HCl (gas)

4) Vibrational spectroscopy of polyatomic molecules
Concepts: group theory, normal modes of vibration; characteristic frequencies; combination modes and overtones. Activities in Raman and IR.
Relation of experiments: (i) the vibrational spectrum of CO_2 and determination of normal modes from first principles and by group theory; (ii) vibrational spectrum of water: solid, liquid and gas; (iii) vibrational spectrum: polyatomic molecules and group theory; Note: Multiple experiments / data collection can be performed in a single day.

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

Bibliography

1. D.A.McQuarrie and J.D.Simon, Physical Chemistry: A Molecular Approach, University Science Books; 1ª. edição (1997).
2. Oswaldo Sala, Fundamentos da Espectroscopia Raman e no Infravermelho; Ed.Unesp, 1ª. Edição (1996).
3. Herzberg, G., Molecular spectra and molecular structure I - spectra of diatomic molecules
4. J. M. Hollas, Modern Spectroscopy, 4ª edição (2004).

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.