



PROGRAMS AND BIBLIOGRAPHY

Subject	
Code	Name
QF530	Introduction to Quantum Chemistry and Molecular Spectroscopy

Vector
OF:S-5 T:004 P:000 L:000 O:000 D:000 HS:004 SL:004 C:004 AV:N EX:S FM:75%

Pre requirement	F 328 *MA311
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Summary

Fundamental notions of spectroscopy and the postulates of quantum mechanics. The particle in a box and electronic structure. The rigid rotor and the rotational spectroscopy of diatomic molecules. The harmonic oscillator and the vibrational spectroscopy of diatomic molecules. Rotational-vibrational spectroscopy of diatomic molecules. Electronic structure, ground and excited states. Photochemistry and photophysics.

Program

- Fundamental notions of spectroscopy and the postulates of quantum mechanics.** The interaction of matter and radiation: absorption, emission, scattering and diffraction. Einstein coefficients, lasers, the transition dipole moment and selection rules. Black-body radiation and de Broglie waves. The postulates of quantum mechanics: wave functions, operators and the computation of properties; the time-dependent and time-independent Schroedinger equations. Applications to the particle in a box and its relation to electronic spectroscopy.
- Rotational-vibrational spectroscopy.** Rotational microwave spectroscopy and fundamentals of instrumentation. The rigid-rotor model, spectra of diatomic molecules and selection rules. Infrared spectroscopy and instrumentation. The harmonic and anharmonic oscillator models. The rotational-vibrational spectrum of diatomic molecules and selection rules. Raman spectroscopy and selection rules.
- Electronic structure.** Instrumentation for UV-vis spectroscopy. The hydrogen atom. Emission and absorption spectra and selection rules. Notions on the Stark and Zeeman effects. The Hamiltonian operator for multi-electronic systems. Spin, the Pauli exclusion principle and Slater determinants. Molecules and the Born-Oppenheimer approximation. Fundamentals of the Hartree-Fock method. The variational principle and the linear combination of atomic orbitals. Application to molecules. The Hückel method and pi systems. Absorption and emission UV-vis spectroscopy. Notions of photophysics and photochemistry.

Bibliography

- D.A.McQuarrie and J.D.Simon, Physical Chemistry: A Molecular Approach, University Science Books; 1a. edição (1997).
- Oswaldo Sala, Fundamentos da Espectroscopia Raman e no Infravermelho; Ed.Unesp, 1ª. Edição (1996).
- G. N. Barrow, Introduction to Molecular Spectroscopy; McGraw-Hill Education, (1962).

Evaluation criteria

Critérios de avaliação definidos pelo Professor, com base no disposto na Seção I – Normas Gerais, Capítulo V – Da Avaliação do Aluno na Disciplina, do Regimento Geral de Graduação. Frequência: 75 % (* O abono de faltas será considerado dentro do previsto no capítulo VI, seção X, artigo 72 do Regimento Geral de Graduação)