

Guia docent de l'assignatura "Espectroscòpia"**2011/2012**

Codi: 102531

Crèdits ECTS: 6

Titulació	Pla	Tipus	Curs	Semestre
2502444 Química	953 Graduat en Química	OB	2	2

Contacte

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Utilització d'idiomes

Llengua vehicular majoritària: anglès (eng)

Algun grup íntegre en anglès: Sí

Algun grup íntegre en català: No

Algun grup íntegre en espanyol: No

Prerequisites

- Teaching, including teaching materials handed over to students, will be in English, hence good communication skills in English are necessary.
- Only students that have passed the basic topics of Fundamentals of Chemistry ("Fonaments de Química") and Experimentation and Documentation ("Experimentació i Documentació") can take Spectroscopy ("Espectroscòpia").
- The course assumes that the student has working knowledge of quantum chemistry; it is thus advisable to have taken (and preferably passed) the Quantum Chemistry ("Química Quàntica") subject.

Objectius i contextualització

In the topic of Spectroscopy the focus is the study of the interaction of electromagnetic radiation and matter, and how this interaction can be used to determine details on the structure of matter. The theoretical foundations that explain the interaction of radiation and matter and predict the structured form of spectra are laid out first, assuming a working knowledge of quantum chemistry. Laser radiation is discussed, as is ubiquitous in current spectroscopy. From there on, different spectroscopic techniques are discussed. For each kind, the structure of the corresponding spectrum is connected to the structural parameters of the molecules using quantitative relations derived from quantum mechanics. A specific focus is made on symmetry as a powerful tool to explain characteristics of certain spectra.

Specific goals of the topic:

- Understand the basics of interaction of electromagnetic radiation with matter.
- Understand the rules that determine the frequency and intensity of a transition.
- Know how to apply this knowledge to be able to solve problems both in qualitative and quantitative aspects.

Competències i resultats d'aprenentatge**1953:E01 - Demostrar que es comprenen els conceptes, els principis, les teories i els fets**

fonamentals de les diferents àrees de la química.

1953:E01.74 - Identificar els principis físics que regeixen les interaccions matèria-radiació.

1953:E02 - Aplicar els coneixements químics a la resolució de problemes de naturalesa quantitativa o qualitativa en àmbits familiars i professionals.

1953:E02.41 - Aplicar els principis físics de les interaccions matèria-radiació a la interpretació qualitativa i quantitativa d'espectres.

1953:E02.42 - Utilitzar els principis físics de les interaccions matèria-radiació per relacionar els senyals dels diferents espectres amb les possibles espècies presents en un determinat sistema químic.

1953:E02.44 - Emprar i generalitzar les relacions entre l'estructura i els mètodes espectroscòpics.

1953:E02.45 - Fonamentar la resposta espectroscòpica en les diferents característiques estructurals.

1953:E06 - Interpretar les dades obtingudes mitjançant mesures experimentals, incloent-hi l'ús d'eines informàtiques; identificar-ne el significat i relacionar les dades amb les teories químiques, físiques o biològiques apropiades.

1953:E06.18 - Manejar programes informàtics, de simulació, entre d'altres, que ajudin a la interpretació anterior.

1953:E09 - Emprar correctament la llengua anglesa en l'àmbit de la química.

1953:E09.10 - Manejar els termes químics més habituals en anglès.

1953:E09.11 - Reconèixer la terminologia espectroscòpica en llengua anglesa.

1953:E09.12 - Reconèixer els termes anglesos de l'estructura química.

1953:E09.21 - Comunicar-se al laboratori en anglès.

1953:T02 - Gestionar l'organització i la planificació de tasques.

1953:T02.00 - Gestionar l'organització i la planificació de tasques.

1953:T03 - Resoldre problemes i prendre decisions.

1953:T03.00 - Resoldre problemes i prendre decisions.

1953:T04 - Obtenir informació, incloent-hi la utilització de mitjans telemàtics.

1953:T04.00 - Obtenir informació, incloent-hi la utilització de mitjans telemàtics.

1953:T05 - Gestionar, analitzar i sintetitzar informació.

1953:T05.00 - Gestionar, analitzar i sintetitzar informació.

1953:T06 - Utilitzar la informàtica per al tractament i presentació d'informació.

1953:T06.00 - Utilitzar la informàtica per al tractament i presentació d'informació.

1953:T07 - Tenir destresa per al càlcul numèric.

1953:T07.00 - Tenir destresa per al càlcul numèric.

1953:T08 - Comunicar-se amb claredat en anglès.

1953:T08.00 - Comunicar-se amb claredat en anglès.

1953:T11 - Raonar de forma crítica.

1953:T11.00 - Raonar de forma crítica.

1953:T12 - Mantenir un compromís ètic.

1953:T12.00 - Mantenir un compromís ètic.

1953:T13 - Aprendre de manera autònoma.

1953:T13.00 - Aprendre de manera autònoma.

1953:T14 - Adaptar-se a noves situacions.

1953:T14.00 - Adaptar-se a noves situacions.

1953:T15 - Proposar idees i solucions creatives.

1953:T15.00 - Proposar idees i solucions creatives.

1953:T18 - Demostrar motivació per la qualitat.

1953:T18.00 - Demostrar motivació per la qualitat.

Continguts

I. Introduction to Spectroscopy

Nature of the electromagnetic radiation. Energy and types of radiation. Electromagnetic spectrum. Spectroscopic techniques. Intensity of spectral lines. Transition dipole moment. Selection rules. Raman Spectroscopy. Selection Rules. Spectral line width. Uncertainty principle. Laser radiation and laser types.

II. Rotational Spectroscopy

Rotation of diatomic molecules. Rigid rotor model. Non-rigid rotor model. Rotation of polyatomic molecules.

III. Vibrational Spectroscopy of Diatomic Molecules

Vibration of diatomic molecules. Harmonic oscillator model. Anharmonicity. Dissociation energy. Rotationa-vibrational coupling. Rovibrational Spectra.

IV. Molecular Symmetry

Symmetry elements and operations. Symmetry point groups. Systematic determination of molecular point group. Reducible and irreducible representations. Symmetry species. Character tables.

V. Vibrational Spectroscopy of Polyatomic Molecules

Vibration of polyatomic molecules. Normal modes of vibration. Types of normal modes. Symmetry of normal modes. Selection rules. Mutual exclusion rule.

VI. Electronic Spectroscopy

Atomic spectroscopy. Spectral terms. Selection Rules. Electronic spectroscopy of diatomic molecules. Vibrational structure. Franck-Condon principle. Electronic spectroscopy of polyatomic molecules. Symmetry considerations. Fluorescence and phosphorescence. Photoelectron spectroscopy.

VII. Magnetic Resonance Spectroscopy

Nuclear and electronic spin. Interaction with a magnetic field. Nuclear magnetic resonance (NMR) spectroscopy. Energy levels. Selection rules. Nuclear shielding. Chemical shift. Spin-spin coupling. Fourier Transform NMR. Radiofrequency pulse. Electron spin resonance. Hyperfine structure.

Lab Sessions

A total of five sessions (4 hours each), plus a sixth session of evaluation:

1. Basic experimental techniques in spectroscopy
2. Vibrational Spectroscopy
3. Electronic Spectroscopy
4. NMR Spectroscopy
5. A Project/Case

Metodologia

The activities belong to three different categories:

Theory Lectures

The lecturer will explain the syllabus to the classroom using blackboard and multimedia material, which will be made available to the students in the "Campus Virtual". These expositive sessions will conform most of the theory lecturing of the syllabus.

Problem-solving Sessions:

A list of graded exercises, classified according to the units of the syllabus, will be made available to all students in the "Campus Virtual" at the beginning of the term. On those lecture hours corresponding to problem-solving, a teaching assistant will solve selected problems, explaining the theoretical foundations, computational details, etc., necessary to solve the exercise and in the process strengthen the concepts explained in the theory lectures.

Lab Sessions

The practical sessions will present the students with the possibility to compute spectroscopic properties of certain molecules using quantum chemistry code or other software, to simulate spectra and also be introduced to basic spectroscopic techniques in a real chemistry lab. It is a goal of the lab sessions to bring up the benefits of a synergy between theoretical and experimental approaches in modern chemistry.

Operationally, the students will be divided in two groups, the composition of which will be known beforehand. Practical sessions for both subgroups will take place simultaneously in different labs under supervision. For all practical sessions, the lab protocol will be made available in the "Campus Virtual", and the students have to bring their own hard copy and read it before the lab session. It is advisable to bring also a personal notebook to write down the results obtained and other annotations. Besides, in experimental lab sessions it is compulsory that students show up with apron and protective goggles.

On appointed days, the students will be summoned to the lab/computer room. At the end of each practical session the students will be given an answer sheet and questionnaire, to be completed individually and turned in before leaving the lab, which will serve the purpose of assessing the level of comprehension of the task just completed and the quality of the results obtained.

Important Note:

Teaching, including all teaching and evaluation materials (e.g. exams, lab report forms) will be given out in English. However, written answers in evaluation materials will be accepted in Catalan and Spanish.

Activitats formatives

Activitat	Hores	ECTS	Resultats d'aprenentatge
Tipus: Dirigides			
Lab Sessions	16	0.64	1953:E02.41 , 1953:E02.42 , 1953:E02.45 , 1953:E09.10 , 1953:E09.12 , 1953:T03.00 , 1953:T05.00 , 1953:T07.00 , 1953:T18.00 , 1953:T15.00 , 1953:T14.00 , 1953:T12.00 , 1953:T11.00 , 1953:T08.00 , 1953:T06.00 , 1953:T04.00 , 1953:E09.21 , 1953:E09.11 , 1953:E06.18 , 1953:E02.44
Problem Solving Sessions	9	0.36	1953:E01.74 , 1953:E09.12 , 1953:T18.00 , 1953:T13.00 , 1953:T11.00 , 1953:T08.00 , 1953:T07.00 , 1953:T03.00 , 1953:T02.00 , 1953:E09.21 , 1953:E09.11 , 1953:E02.42 , 1953:E02.45 , 1953:E06.18 , 1953:E09.10 , 1953:E02.44 , 1953:E02.41
Theory Lectures	29	1.16	1953:E01.74 , 1953:E02.41 , 1953:E02.42 , 1953:E02.45 , 1953:E09.10 , 1953:E09.12 , 1953:T05.00 , 1953:T11.00 , 1953:T13.00 , 1953:T08.00 , 1953:T04.00 , 1953:E09.11 , 1953:E06.18 , 1953:E02.44
Tipus: Supervisades			
Case Preparation	6	0.24	1953:E01.74 , 1953:T07.00 , 1953:T06.00 , 1953:T05.00 , 1953:T04.00 , 1953:T03.00 , 1953:T02.00 , 1953:E09.21 , 1953:E09.12 , 1953:E09.11 , 1953:T18.00 , 1953:T15.00 , 1953:T14.00 , 1953:T13.00 , 1953:T12.00 ,

1953:T11.00 , 1953:T08.00 , 1953:E02.42 , 1953:E02.44 , 1953:E02.45 , 1953:E09.10 , 1953:E06.18 , 1953:E02.41			
Tipus: Autònomes			
Personal Study	70	2.8	1953:E01.74 , 1953:T13.00 , 1953:T11.00 , 1953:T07.00 , 1953:T05.00 , 1953:T04.00 , 1953:T03.00 , 1953:T02.00 , 1953:E09.12 , 1953:E09.11 , 1953:E02.42 , 1953:E02.44 , 1953:E02.45 , 1953:E09.10 , 1953:E06.18 , 1953:E02.41
Problem Solving	9	0.36	1953:E01.74 , 1953:E09.10 , 1953:E09.12 , 1953:T15.00 , 1953:T13.00 , 1953:T11.00 , 1953:T08.00 , 1953:T07.00 , 1953:T05.00 , 1953:T04.00 , 1953:T03.00 , 1953:T02.00 , 1953:E09.11 , 1953:E06.18 , 1953:E02.41 , 1953:E02.42 , 1953:E02.45 , 1953:E02.44

Avaluació

The evaluation is based on a "continuous evaluation" scheme, comprising the following items:

1. A certain number of short individual exercises, spread out along the semester, which will be proposed, done and returned in situ 15%
2. Lab reports, turned in at the end of each practical session 10%
3. Solve a given "Case": working in groups of 4-5 individuals, the students will have to work out, using quantum chemistry software and experimental techniques as needed, detailed spectroscopic properties of proposed molecules, present their case in a short oral presentation, and answer a few questions from the evaluators. The grade will reflect both the quality of the results and presentation (same for all members), and the individual responses of each student 15%
4. Two partial written exams, covering approximately one-half of the syllabus each and to be held on dates and times known at the time of enrolling. A minimum score of 4 /10 is required in each for them to count towards the final grade. Each of these tests will count towards 30% of the final grade. $2 \times 30\% = 60\%$

A final exam, of the same format as the above, which will only be compulsory for students who have not scored 4/10 in both partial exams above. This exam will be longer, divided in two halves matching the contents of the first set of tests. The student is required to take at least the part where s/he did not attain 4/10. Students wishing to improve their score can take this exam too, whole or piecewise. The final grade in this case is that of the final exam -if this is higher-or the average between the final and the partial. Note that it is possible to lower the grade in this way 60%

To pass the subject, students need to attain sufficient proficiency in the practical and theoretical aspects of the topic. The final grade is obtained by adding the following two contributions, (a) and (b), provided that both are 4/10 or better:

1. Practical aspects: items (2)+(3)
2. Theoretical aspects: Item (4)

The topic is passed with a grade of 5/10. Note that lab attendance is compulsory. For grading purposes, a student will be considered as non-evaluable ("no presentat"), if any of the following applies:

1. has not attended any lab session without motive
2. cannot achieve a grade of 5/10 with his/her own evaluation items, and could not achieve it with the same items even if s/he had achieved in those the highest grade.

Activitats d'avaluació

Activitat	Pes	Hores	ECTS	Resultats d'aprenentatge
Case Presentation	15%	1	0.04	1953:E09.10 , 1953:E09.11 , 1953:E09.12 , 1953:T02.00 , 1953:T05.00 , 1953:T04.00 , 1953:T03.00 , 1953:E09.21 , 1953:T06.00 , 1953:T18.00 , 1953:T15.00 , 1953:T14.00 , 1953:T11.00 , 1953:T08.00 , 1953:T07.00
Final Exam	60%	4	0.16	1953:E01.74 , 1953:E02.41 , 1953:E02.42 , 1953:E02.44 , 1953:E09.12 , 1953:T07.00 , 1953:T12.00 , 1953:T15.00 , 1953:T13.00 , 1953:T11.00 , 1953:T03.00 , 1953:E09.11 , 1953:E09.10 , 1953:E02.45
Lab Reports	10%	1	0.04	1953:E02.41 , 1953:E02.42 , 1953:E02.44 , 1953:E09.11 , 1953:E09.21 , 1953:T07.00 , 1953:T12.00 , 1953:T18.00 , 1953:T15.00 , 1953:T11.00 , 1953:T05.00 , 1953:E09.12 , 1953:E09.10 , 1953:E06.18 , 1953:E02.45
Partial Exams	60%	4	0.16	1953:E01.74 , 1953:E02.41 , 1953:E02.42 , 1953:E02.45 , 1953:E09.11 , 1953:T03.00 , 1953:T11.00 , 1953:T13.00 , 1953:T15.00 , 1953:T12.00 , 1953:T07.00 , 1953:E09.12 , 1953:E09.10 , 1953:E02.44
Turned in Exercises	15%	1	0.04	1953:E02.41 , 1953:T18.00 , 1953:T15.00 , 1953:T12.00 , 1953:T11.00 , 1953:T07.00 , 1953:T03.00 , 1953:E02.44 , 1953:E02.45 , 1953:E09.10 , 1953:E09.12 , 1953:E09.11 , 1953:E02.42

Bibliografia

Basic Texts:

- P. Atkins, J. de Paula, Atkins' Physical Chemistry, 8th Ed., Oxford University Press, 2005
- C. N. Banwell, E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th Ed., McGraw Hill, 1994
- J. M. Hollas, Modern Spectroscopy, 4th Ed., John Wiley & Sons, 2004 (Does not cover magnetic resonance)

Specialized Texts and Monographies:

- P. Atkins, R. Friedman, Molecular Quantum Mechanics, 5th Ed., Oxford University Press, 2011
- A. Vincent, Molecular Symmetry and Group Theory, 2nd Ed., John Wiley & Sons, 2001
- P. J. Hore, Nuclear Magnetic Resonance, Oxford Chemistry Primers, Oxford University Press, 1995