Determinació Estructural 2014/2015

Codi: 102532
Crèdits: 6

Titulació	Tipus	Curs	Semestre
2502444 Química	OB	3	1

Professor de contacte

Nom: Jordi Hernando Campos
Correu electrònic: Jordi.Hernando@uab.cat

Utilització de llengües

Llengua vehicular majoritària: anglès (eng)
Grup íntegre en anglès: Sí
Grup íntegre en català: No
Grup íntegre en espanyol: No

Equip docent

Juli Real Obradors

Prerequisits

- All teaching, including teaching materials handed out to the students, will be in English. Therefore, good communication skills in English are necessary.
- Only students who have passed the 2nd-year subject "Spectroscopy" ("Espectroscòpia") are recommended to take "Structural Determination".
- The course assumes that the student is familiar with the basic concepts of organic and inorganic chemistry. Therefore, the students are expected to have taken the 2nd-year subjects "Estructura i Reactivitat dels Compostos Orgànics" and "Química dels Elements".

Objectius

This course aims at providing the students with basic tools for the analysis of the spectroscopic data of organic and inorganic molecular compounds, thus enabling the students to elucidate their structure. Various spectroscopic and spectrometric techniques will be considered (mass spectrometry and UV-vis, infrared and nuclear magnetic resonance spectroscopies), though most efforts will be devoted to the analysis of NMR data.

Specific goals of this subject are:

- Introduce the mass spectrometry technique and review basic concepts of UV-vis, IR and NMR spectroscopies covered by the 2nd-year subject "Spectroscopy".
- Introduce advanced concepts in NMR spectroscopy.
- Use this knowledge to undertake the analysis of mass, UV-vis, IR and 1D NMR spectra of organic and inorganic molecular compounds.
- Elucidate the structure of those compounds based on their spectroscopic data.

Competències

- Adaptar-se a noves situacions.
- Aplicar els coneixements químics a la resolució de problemes de naturalesa quantitativa o qualitativa en àmbits familiars i professionals.

- Aprendre de manera autònoma.
- Comunicar-se amb claredat en anglès.
- Demostrar motivació per la qualitat.
- Emprar correctament la llengua anglesa en l'àmbit de la química.
- Gestionar l'organització i la planificació de tasques.
- Gestionar, analitzar i sintetitzar informació.
- 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.
- Manejar instruments i material estàndard en laboratoris químics d'anàlisi i síntesi.
- Mantenir un compromís ètic.
- Obtenir informació, incloent-hi la utilització de mitjans telemàtics.
- Proposar idees i solucions creatives.
- Raonar de forma crítica.
- Reconèixer i analitzar problemes químics i plantejar respostes o treballs adequats per a resoldre'ls.
- Resoldre problemes i prendre decisions.
- Utilitzar la informàtica per al tractament i presentació d'informació.

Resultats d'aprenentatge

1. Adaptar-se a noves situacions.
2. Analitzar problemes químics i planejar a nivell espectroscòpic respostes o treballs adequats per a la seva resolució, utilitzant models moleculars i fonts bibliogràfiques.
3. Aprendre de manera autònoma.
4. Avaluar la millor metodologia espectroscòpica per a la resolució d'un problema estructural.
5. Avaluar les capacitats de la informació continguda a les xarxes en línia.
6. Comunicar-se amb claredat en anglès.
7. Demostrar motivació per la qualitat.
8. Examinar bases de dades espectroscòpiques i altres dades bibliogràfiques relacionades.
9. Gestionar l'organització i la planificació de tasques.
10. Gestionar, analitzar i sintetitzar informació.
11. Innovar mètodes per adequar-los a la interpretació d'una estructura molecular concreta.
12. Interpretar les dades obtingudes en les mesures experimentals per expressar una estructura química.
13. Interrelacionar bases de dades i programes de càlcul per determinar una estructura.
14. Manejar els termes químics més habituals en anglès.
15. Mantenir un compromís ètic.
16. Obtenir informació, incloent-hi la utilització de mitjans telemàtics.
17. Proposar idees i solucions creatives.
18. Raonar de forma crítica.
19. Reconèixer i analitzar problemes químics estructurals en compostos orgànics i inorgànics.
20. Reconèixer la terminologia anglesa en les bases de dades bibliogràfiques i la informació en línia.
21. Resoldre problemes i prendre decisions.
22. Utilitzar els mètodes espectroscòpics [IR, UV-VIS, RMN (1 H, 13 C) i EM] per a la resolució de problemes de naturalesa quantitativa o qualitativa en l'àmbit de l'estructura i les relacions intra- i intermoleculars.
23. Utilitzar la informàtica per al tractament i presentació d'informació.

Continguts

1. Introduction to Mass Spectrometry (MS)

Background and the experimental method. Spectral resolution. Isotope analysis. Fragmentation processes: homolytic and heterolytic bond cleavage. Fragmentation patterns associated to specific functional groups. Examples.

2. Basic concepts in Electronic (UV-Vis), Infrared (IR) and Nuclear Magnetic Resonance (NMR) Spectroscopies.

The experimental methods. UV-vis chromophores in organic molecules. IR absorptions of organic functional groups and interpretation of IR spectra. Functional group charts (IR). Basic aspects of NMR spectra: chemical shifts, spectral ranges and referencing.

3. ^{1}H NMR: the chemical shift.

Shielding mechanisms. Topical relationships and molecular symmetry. Other factors influencing the chemical shift: magnetic anisotropy, solvent effects. Correlations: hydrogens linked to carbon, hydrogens linked to other nuclei. Spectral simulations. Examples.

4. ^{1}H NMR: spin-spin coupling.

Basic concepts on spin-spin interaction, coupling constants and multiplicity patterns. The Karplus equation. Spin systems: the $\Delta\nu/J$ ratio, first and second order spectra. Heteronuclear couplings. Examples.

5. ^{1}H NMR: analysis of the spectra.

Time-dependent phenomena. Methods of analysis. Simplification of spectra: changing the magnetic field, spin decoupling, shift reagents. Cross-relaxation and the nuclear Overhauser effect (nOe). Introduction to 2D NMR spectroscopy. Examples.

6. ^{13}C NMR.

Overview. Recording methods (broad band, off-resonance, DEPT). Chemical shifts: additivity and spectral simulations. Spin-spin couplings. Analysis of the spectra. Examples

7. NMR of other nuclei.

^{1}H NMR in inorganic compounds, including metal complexes. ^{31}P NMR, ^{19}F NMR, ^{14}N and ^{15}N NMR. Metal complexes: multinuclear NMR.

8. Structural determination.

Combined application of the spectroscopic techniques. Examples.

Metodologia

Two different types of activities will be developed in the classroom:

Theory Lectures

The lecturer will explain the contents of the course to the classroom using blackboard and multimedia material, which will be made available to the students in the "Campus Virtual". After a set of lecture sessions taking place during the initial weeks to introduce basic concepts, the rest of the theory lectures will be based on a "problem-based learning" approach.

Problem-solving Sessions

A set of exercises will be made available to all students in the "Campus Virtual" at the beginning of the course. Several of these will be discussed by a teaching assistant during the problem-solving sessions.

Alternatively, students will be required to solve spectroscopic exercises during these sessions, for which a note will be given.

Important Note

Teaching, including all teaching and evaluation materials (e.g. slides, problems, exams), will be given in English. Students are encouraged to use English as well when answering evaluation materials or communicating to the professors. In spite of this, the use of Catalan and Spanish will also be accepted in both cases.

Activitats formatives

Títol	Hores	ECTS	Resultats d'aprenentatge
Tipus: Dirigides			
Problem-solving Sessions	11	0,44	4, 6, 7, 8, 10, 11, 12, 13, 14, 15, 17, 18, 19, 21, 22
Theory Lectures	38	1,52	4, 5, 6, 7, 8, 11, 12, 13, 14, 15, 17, 18, 19, 21, 22
Tipus: Autònomes			
Personal study	29	1,16	3, 5, 7, 9, 10, 14, 15, 16, 18, 19, 20
Problem Solving	58	2,32	1, 3, 4, 5, 7, 8, 9, 10, 11, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23

Avaluació

1. In principle, the overall grade will be broken down as follows:

Problems solving (25%) + 1st Midterm Exam (25%) + 2nd Midterm Exam (50%) = 100%

The evaluation of students will comprise the following items:

- Problems solving: A number of short exercises will be periodically handed out to the students. They will be either done during class or handed in to the lecturer after a specified period of time (typically, one week). A grade will be given to each exercise, and that with the lowest note will be excluded from evaluation. The average note of the remaining exercises will account for 25% of the overall grade of the course.
- Written exams: Two midterm exams will be held during the course and they will account for 25% and 50% of the overall grade of the course, respectively.

To pass the subject, students must fulfill both of the following requisites:

A) The weighted average note of the two partial exams must be at least 5/10.

B) The overall grade (problems + MT1 + MT2) should be at least 5/10.

2. A final exam is also scheduled and will be compulsory for those with a weighted average score for the two partial exams lower than 5/10. Those with a passing grade but who wish to improve their note may also take the final exam.

For those students taking the final exam, the overall note will be computed as follows:

Problems solving (25%) + 1st Midterm Exam (5%) + 2nd Midterm Exam (10%) + Final Exam (60%) = 100%

The formula will apply to all students who have taken the final exam, regardless of whether the new note is higher or lower than the original.

To pass the subject, students must fulfill both of the following requisites:

A) The weighted average mark of all three exams must be at least 5/10.

B) The overall grade (problems + MT1 + MT2 + Final Exam) should be at least 5/10

Students taking less than 1/3 of the evaluation items will be graded as "no presentat".

Activitats d'avaluació

Títol	Pes	Hores	ECTS	Resultats d'aprenentatge
Exams	75%	4	0,16	1, 3, 4, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22
Problem Solving	25%	10	0,4	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23

Bibliografia

a) Text books

- D.H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, McGraw-Hill, London, 2007.
- R. Silverstein, F.X. Webster, D.J. Kiemle, Spectrometric Identification of Organic Compounds, Wiley, New York, 2005.
- P. Crews, J. Rodriguez, M. Jaspars, Organic Structure Analysis, Oxford University Press, New York, 2009.

b) Problems

- L.D. Field, S. Sternhell, J.R. Kalman, Organic Structures from Spectra, Wiley, Chichester, 2008.

c) Tables

- E. Pretsch, P. Bühlmann, C. Affolter, A. Herrera, R. Martínez, Determinación estructural de compuestos orgánicos, Springer, Barcelona, 2002.
- E. Pretsch, P. Bühlmann, M. Badertscher, Structure Determination of Organic Compounds, Springer, Berlin, 2009.