

Subject:	Magnetic Techniques: Spectroscopies and Imaging
Semester:	Spring
Credits ECTS:	2,5
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Department / Faculty:	Inorganic Chemistry Faculty of Chemistry, UB

Objectives:

- To introduce the didactic and pedagogical basis of the spectroscopic techniques to the students.
- To study the models and principles of the magnetic spectroscopy and imaging techniques to the student.
- To present the interest and applications of the magnetic spectroscopy and imaging techniques.
- *The specific competences the student will acquire are:*
- Basic knowledge of NMR and EPR spectroscopies.
- To know the specific methods of each spectroscopy and their application limits
- in the Nanoscience field.
- To manage with accurate criteria the spectroscopic principles.
- To interpret the spectra and to correlate the results with the structure and properties.

Recommendations / Requisites

Bachelors degree (B.S.) in Physics, Chemistry or Pharmaceutics and a general knowledge of the basic principles of Quantum Chemistry.

Contents:

Topic-1: Introduction. Relevance of the spectroscopy techniques in the Nanoscience field. Main magnetic spectroscopies: Nuclear Magnetic Resonance (NMR) and Electronic Paramagnetic Resonance (EPR).

Topic-2: Magnetic properties of the nucleus. Energy level and resonant transitions. Experimental methods. Relaxation process. Nuclear Magnetic Resonance Parameters: chemical shift, coupling constants and intensity of the signals.

Topic-3: Monodimensional Nuclear Magnetic Resonance of ^1H and ^{13}C . Chemical shifts and their relation with the molecular structure. Empiric Correlations. Exchange processes. Symmetry and Chemical shift. Coupling and decoupling phenomena.

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Master Community: <http://campusvirtual.ub.edu/course/view.php?id=427>

Website: <http://www.ub.edu/nanotec/>

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Topic-4: Monodimensional Nuclear Magnetic Resonance of other nucleus with $I = 1/2$. Isotopomers. Nuclear Magnetic Resonance of nucleus with quadrupolar momentum.

Topic-5: Two-dimensional NMR. Multipulse sequences. Homocorrelations $^1\text{H}-^1\text{H}$: structural information and exchange processes. Heterocorrelations $^1\text{H}-^{\text{X}}\text{X}$ ($^{\text{X}}\text{X} = ^{13}\text{C}$, ^{31}P , etc).

Topic-6: Utility of NMR in Nanosystems characterization. Imaging techniques. Examples.

Topic-7: Basis of Electronic Paramagnetic Resonance. Zeeman Hamiltonian. Hamiltonian of electron-nucleus interactions. Structural information. Application to organic compounds with one free electron. Examples.

Topic-8: Spin Hamiltonian. Free electron case. Isotropic and anisotropic systems. g -values. Hyperfine splitting. Electronic delocalization.

Topic-9: Polyelectronic systems. Zero-field splitting Hamiltonian. Isotropic and anisotropic systems. Examples.

Topic-10: EPR of polynuclear compounds. Examples of discrete and low dimensional systems.

Topic -11: Time-dependent phenomena. Relaxation. Electronic delocalization. EPR of mixed valence polynuclear compounds.

Topic -12: Utility of EPR for the characterization of Nanosystems. Examples.

Plan:

Lectures: 23 hours.

Independent work: 14 hours.

Study: 32 hours.

Bibliography

- 1) Ebsworth, E.V.A, Rankin, D.W.H., Cradock, S. *Structural Methods in Inorganic Chemistry* (2nd ed.). Blackwell Scientific, 1991.
- 2) Hore, P.J. *Nuclear Magnetic Resonance*, Oxford University Primeros, 32, 1995.
- 3) Drago, R.S. *Physical Methods for Chemists*. Saunders Publishing, 1977.
- 4) Pretsch, E. Bühlmann, P. Affolter, C. Herrera, A. Martínez, R. *Determinación Estructural de Compuestos Orgánicos*. Springer, 2001.
- 5) Weil, J. A.; Bolton, J. R.; Wertz, J. E. *Electron Paramagnetic Resonance*. John Wiley, New York, 1994.