האוניברסיטה העברית בירושלים
THE HEBREW UNIVERSITY OF JERUSALEM

The Hebrew University of Jerusalem

Syllabus

Fundamentals of NMR - 69149

Last update 24-09-2024

HU Credits: *2*

Degree/Cycle: *2nd degree (Master)*

Responsible Department: *Chemistry*

Academic year: *0*

Semester: *2nd Semester*

Teaching Languages: *English*

Campus: *E. Safra*

Course/Module Coordinator: *Daphna Shimon*

Coordinator Email: *daphna.shimon@mail.huji.ac.il*

Coordinator Office Hours: *I am flexible, email to arrange a meeting*

Teaching Staff:

Dr. Daphna Shimon

Course/Module description:

Course about the basics of NMR spectroscopy from a chemical physics perspective

Course/Module aims:

Learning outcomes - On successful completion of this module, students should be able to:

1. The student will be able to look at an NMR spectrometer and identify the different parts.

2. The student will know how to run a simple NMR experiment, and will know what to do at each stage for the experiment to be successful.

3. The student will be able to follow the magnetization vector through an NMR experiment.

4. The student will be able to describe an NMR experiment with quantum mechanics.

Attendance requirements(%):

None

Teaching arrangement and method of instruction:

Course/Module Content:

1. Classical description of NMR:
Motion of charged particles. Magnetic moments and magnetic fields. Nuclear magnetizations. Classical motion of the spins. Rf irradiation of the spins and the rotating frame.

2. Principles of pulsed NMR:
The pulsed NMR experiment (square pulses). Quadrature detection in the rotating frame. Fourier analysis, discrete sampling, and fast Fourier transform. Effects of relaxation and the Bloch equations. NMR line shapes and the phase of spectral peaks. Broadband irradiation, selective irradiation, composite pulses. Artifacts and phase cycling. Signal-to-noise in pulsed NMR.

3. The basic NMR spectrometer:
Magnets, shims, spinning, locking, probe, tuning/matching. Review of electronics. NMR detection and digitization.

4. MR interactions:
The chemical shift, J coupling, dipolar interactions in solutions. NMR spectra of organic molecules & decoupling. Solid State NMR interactions and line Shapes. Averaging of anisotropic couplings in solution NMR. Averaging Techniques in Solids. The classical description of single-spins.

5. Pulse sequences for 2D spectroscopy:
Classical description of simple two-spin systems. Polarization transfer methods. Some well known 2D experiments for solution NMR.

6. Short introduction to EPR (and electron-nuclear interactions), Solid state DNP and MRI.

7. The quantum mechanics of NMR (only if time permits):
The spin wave function, the density matrix, angular momentum operators and expectation values. Descriptions for static solid-state NMR.

Required Reading:
none

Additional Reading Material:
Keeler, Understanding NMR Spectroscopy - http://www-keeler.ch.cam.ac.uk/lectures/
Jacobsen, NMR Spectroscopy Explained
Levitt, Spin Dynamics
Apperley, Harris, and Hodgkinson, Solid-state NMR : Basic Principles & Practice

Grading Scheme:
Essay / Project / Final Assignment / Home Exam / Referat 85 %
Submission assignments during the semester: Exercises / Essays / Audits / Reports / Forum / Simulation / others 15 %

Additional information:

At the end of the course the students will have to write an essay. More details will be given during the semester.