Chemistry/Biochemistry 146b
Advanced NMR Spectroscopy

Time and Place: MW 2:00 PM–3:20 PM, Place TBA.

Instructor: Tom Pochapsky (x62559, pochapsk@brandeis.edu). Office hours 10-11 AM on class days, Rosenstiel 655.


Course Description: The principles behind modern nuclear magnetic resonance (NMR) theory and applications will be described. The student is expected to have had successfully completed college courses in general chemistry, physics and calculus.

Work load: It is expected that this course will require at least three hours of effort for each hour of class time (i.e., 12 hours per week total). This includes completion of homework assignments and reading.

Learning goals: The course is designed to introduce students with backgrounds in the physical and life sciences to the theory and applications of NMR spectroscopy, including two- and three-dimensional NMR methods, solid state NMR and MRI (magnetic resonance imaging). While no prior knowledge is assumed other than what is provided by the above-mentioned college courses, the student will be introduced to classical and quantum mechanical operator descriptions of the NMR experiment, Fourier transformation of time-domain NMR data, radiofrequency pulse excitation, and coherence selection methods. As time permits, “hands-on” experience will be provided, and realistic data processing and manipulation demos will be available. It is expected that after successful completion of the course, the student will gain competencies in NMR data acquisition, processing and analysis.

Mathematica exercises: Homework and demo packages used throughout the semester will require you to have access to the Mathematica program, for which the University has a site license. Computers around campus have the program mounted for student use, or if you are working in a laboratory, you should make sure a lab computer has the software mounted.

Homework and Exams: A weekly problem set will be assigned each Thursday, due the following Thursday. Two exams will be given, a mid-term and a final. The mid-term is tentatively scheduled for Weds, Oct 16th, during class. The final will be given at the Registrar-assigned time during finals week.
**Practical sessions:** Within limitations of time, course enrollment and instrument availability, the director of the NMR facility, Dr. Susan Sondjej Pochapsky, will provide some practical experience with principles discussed in the course using the MR 400 MHz NMR in the basement of Shapiro Science Center.

A list of topics to be covered in order of appearance:

1) What is spectroscopy?
2) Elementary aspects of NMR - chemical shift
3) Dipolar and scalar coupling
4) Time scales in NMR
5) Nuclear relaxation I
6) Fourier transform NMR
7) Relaxation II - the nuclear Overhauser effect
8) Mechanisms of relaxation
9) Polarization transfer
10) Multidimensional NMR I
11) The spin operator formalism
12) Density operators and product operators
13) Coherence evolution using product operators
14) Homonuclear 2D experiments
15) Spin-locking fields (ROESY, TOCSY) and the Hartmann-Hahn condition
16) Indirect detection of insensitive nuclei: HMQC, HSQC
17) Coherence selection - phase cycling
18) Coherence selection - pulsed field gradients
19) Multistep coherence transfers
20) Indirect detection heteronuclear relaxation experiments
21) Selective excitation, shaped pulses and diffusion measurements
22) Solid state NMR
23) Imaging