

CHEM 390

Special Topics in Chemistry, Honors
Nuclear Magnetic Resonance: Fundamentals and Applications

M,W 1:00 – 2:15 pm, 2074 Malott Hall

Instructor: Prof. Misha Barybin, 1025 Malott Hall, mbarybin@ku.edu

Office Hours Tuesdays, 12:30 – 3:30 pm at Nunemaker Center (Room 101) or by appointment

Suggested Text P. J. Hore, *Nuclear Magnetic Resonance, 2nd Edition*, OXFORD University Press, 2015, 112 pp. ISBN 978-0-19-870341-9
(not required)

Reading Assignments Reading assignments will be given in class and will include journal articles, textbook excerpts, and other hard copy or electronically accessible materials.

Problem Sets Problem sets will be given every week to support lectures. Sources other than lecture notes and assigned reading may have to be consulted to work on certain problems.

<u>Grading:</u>	Homework problem sets	30%
	In-class presentation	10%
	Two take-home exams	2×20%
	NMR Lab Project	15%
	In-class discussion participation	5%

Special Needs: The KU Office of Student Access Services (SAS), part of the Academic Achievement & Access Center (AAAC), coordinates accommodations and services for all eligible students. If you have a disability for which you wish you request accommodations please contact AAAC. The AAAC office is located in Strong Hall, Room 22; their phone number and email address are (785)864-4064 (V/TTY) and achieve@ku.edu, respectively. Information about their services can be found at <http://access.ku.edu>. In addition, I would appreciate if students with special needs notify me privately ASAP to ensure timely arrangement of special accommodations.

Course Website: All students enrolled in CHEM 390 have been granted access to the BLACKBOARD site for this course at <http://courseware.ku.edu>. Be sure you are able to access this site to view information pertaining to the course including electronic handouts, announcements, etc. You will be prompted to enter your KU Online ID and Password to access the course materials. If you have trouble accessing the website, please let Dr. Barybin know as soon as possible.

Academic Misconduct: I expect all of you to adhere to high standards of personal and scientific integrity and sincerely hope that we will not have reasons to deal with this issue. After all, any science is not worth much without honest reporting of findings, and the proper authorship attribution (including any materials harvested from the internet!). “The following policy ... defines a uniform approach to acts of academic misconduct involving students in courses offered by the College of Liberal Arts and Sciences.

Academic integrity requires the honest performance of academic responsibilities by students. Academic responsibilities include, but are not limited to, the preparation of assignments, reports and term papers, the taking of examinations, and a sincere and conscientious effort by students to abide by the policies set forth by instructors. Any subversion or compromise of academic integrity thus constitutes academic misconduct. Examples of misconduct include (among others) falsification, unauthorized assistance with or plagiarism of reports, term papers, research papers or other written documents; giving or receiving unauthorized aid on examinations; disruption of classes; the offering of gratuities or favors in return for grades,” etc. Please see the webpage <https://documents.ku.edu/policies/governance/USRR.htm#art2sect6> for more info on this issue.

Any assignments turned in for credit must represent your own work. Any incidence of academic misconduct will be pursued to the fullest extent in accordance with the University policy, as described in the student handbook (see the website above). At a minimum, this includes receiving zero credit for the work in question for any party involved. Additional penalties may include a grade of “F” for the entire course, as well as suspension or even expulsion from the University. If you have questions about what constitutes academic misconduct, please see me and/or consult the student handbook.

Diversity Statement: Students in this course are expected to speak up and participate during class meetings. Because the class represents a diversity of individual backgrounds and experiences, every student in this class must demonstrate respect and positive professional regard for their peers.

KU Policy on Weapons: The University of Kansas adopted on July 1, 2017 its Policy on Weapons, as required by the Board of Regents. Individuals who choose to carry concealed handguns **are solely responsible to do so in a safe and secure manner in strict conformity with [state and federal laws](#) and the [KU Weapons Policy](#)**. Safety measures outlined in the KU Weapons Policy specify that a concealed handgun:

- Must be under the constant control of the carrier.
- Must be out of view, concealed either on the body of the carrier, or backpack, purse, or bag that remains under the carrier’s custody and control.
- Must be in a holster that covers the trigger area and secures any external hammer in an un-cocked position.
- Must have the safety on, and have no round in the chamber.

A few class sessions will take place in KU NMR Lab facilities where carrying a variety of self-defense weapons is restricted due to potentially dangerous interactions thereof with a strong magnetic field. During these activities, students will be expected to leave belongings, such as backpacks and purses, away and unattended for prolonged periods. Students who choose to carry a concealed handgun or other means of self-defense should plan accordingly prior to beginning these class sessions. The university does not provide appropriate secured storage for concealed handguns or any other weapons. Individuals who violate the KU weapons policy may face disciplinary action under the appropriate university code of conduct, including dismissal from the course.

Important Note 1. The issue of digital plagiarism has raised concerns about ethics, student writing experiences, and academic integrity. KU subscribes to a digital plagiarism detection program, which may be used to check papers submitted in this course. You may be asked to submit your papers in a digital format (e-mail attachment) so that your paper can be checked against Web pages and databases of existing papers. Although you may never have engaged in intentional plagiarism, many students do incorporate sources without citations; this program can alert me to your academic needs. In addition, any exams and or papers may be photocopied at the discretion of the instructor without the knowledge or consent of the students.

Important Note 2. Course materials prepared by the instructor, together with the content of all lectures and review sessions are the property of the instructor. Video and audio recording of lectures and review sessions without the consent of the instructor is prohibited. Upon request, the instructor may grant permission to audio tape lectures, on the condition that these audio tapes are only used as a study aid by the individual making the recording. Unless explicit permission is obtained from the instructor, recordings of lectures and review sessions, as well as electronic copies of the instructor's lecture notes, may not be modified and must not be transferred or transmitted to any other person, whether or not that individual is enrolled in the course.

TENTATIVE LECTURE TOPICS (subject to minor changes)

1. In-depth account of NMR principles illustrated by examples for nuclei other than ^1H and ^{13}C
 - A. Bulk magnetization, energy and populations, sensitivity, Larmor frequency
 - B. NMR excitation and detection, Fourier transform, FID, pulses and pulse sequences
 - C. Timescales, chemical shielding, the PPM scale, J -coupling
 - D. Data processing: sensitivity and resolution enhancement
 - E. Structure determination: trends in chemical shifts and coupling constants, satellites, differentiation of chemical shifts and scalar couplings
 - F. Relaxation, measurement of T_1 and T_2
 - G. Determination of thermodynamic and kinetic parameters by NMR, dynamic processes
 - H. Problem solving seminar
2. 2-D NMR Spectroscopy
 - A. The assignment problem and correlation maps
 - B. Interpretation of COSY, TOCSY, ROESY, TROSY, HMQC, HSQC, NOESY, and INADEQUATE correlation maps
 - C. Selected application examples
 - D. Problem solving seminar
3. NMR of paramagnetic substances in solution
 - A. Theory and principles
 - B. Lanthanide shift reagents
 - C. Investigation of structural and electronic equilibria by paramagnetic NMR
 - D. Biochemical applications
 - E. Problem solving seminar
4. Solid State NMR
 - A. Nuclear interactions in the solid state
 - B. Shielding anisotropy, principle axis system, and dipolar splitting
 - C. Magic angle spinning and cross polarization
 - F. Pharmaceutical and materials applications
 - G. Problem solving seminar
5. Fundamentals of Magnetic Resonance Imaging
 - A. Basics of MRI: physical principles and instruments
 - B. Modern variations of MRI
 - C. Metal complexes as contrast agents for MRI: metal and ligand requirements, recent advances, mechanism of action
 - D. Problem solving seminar
6. Other topics of students' choice may be covered as time permits.

About Professor Misha Barybin

Born and raised in Moscow, Russia, Dr. Barybin moved to the United States in 1994, after pursuing his undergraduate studies at Higher College of Chemistry of the Russian Academy of Sciences. He earned his Ph.D. in Chemistry from the University of Minnesota in 1999. Following a two-year postdoctoral stint at MIT, Dr. Barybin joined the faculty of KU's Department of Chemistry in 2001. Professor Barybin's research interests and accomplishments are at the interface of synthetic organometallic, physical inorganic, and materials branches of Chemistry. In particular, his research group is involved in developing new molecular and supramolecular platforms for charge delocalization and transport at the nanoscale that are relevant to molecular electronics. During his career at KU, Professor Barybin has taught twelve different courses, including Honors Fundamentals of Chemistry I & II. He is a recipient of *the 2016 Grant K. Goodman Undergraduate Mentor Award* (KU College of Liberal Arts and Sciences), *the 2015 Outstanding Honors Advisor Award* (University Honors Program), *the 2014 J. Michael Young Academic Advisor Award* (KU College of Liberal Arts and Sciences), *the 2011 Outstanding Educator Award* (KU Mortar Board Honor Society), and *the 2010 Byron Alexander Graduate Mentor Award* (KU College of Liberal Arts and Sciences). Dr. Barybin has been a Faculty Fellow at the University Honors Program since 2013.