CHEM 751: SPECIAL TOPICS IN PHYSICAL CHEMISTRY

Nuclear Magnetic Resonance Spectroscopy: Foundations and Applications

TR 900-1015, Bil 242

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OFFICE: Bilger 241

OFFICE HOURS: By appointment

This Special Topics course will be a primer on NMR spectroscopy, focusing on theoretical and practical foundations that will provide you with the tools to apply this powerful methodology to a diverse and complex range of systems. We will follow (roughly) the material in the Keeler textbook. The class time will be used for lectures, group problem-solving (review of homework), and short quizzes. At the end of the semester, you will demonstrate your new and hopefully growing knowledge of NMR in the Final Project.

PREREQUISITES: Successful completion of courses in quantum mechanics (CHEM 352 or equivalent) and sophomore-level physics (PHYS 170-272 or equivalent).

- Assumes prior knowledge (of NMR) from undergraduate coursework (e.g., sophomore organic, analytical chemistry or instrumental analysis).
- Assumes familiarity with dot products, as well as vector (or “cross”) products.
- Assumes familiarity with the basics of quantum mechanics, such as eigenvalues, eigenfunctions, angular momentum operators, Hamiltonians, and the Schrodinger Equation.
- It is helpful to have some knowledge of matrix algebra (but not essential).


- Book is available at Amazon and also Wiley’s website.
- Book includes a URL for the solutions to the end-of-chapter problems.
- 2nd edition is VERY similar to the 1st edition, so you can probably use either. However, problem sets & reading correspond to the 2nd edition, and the responsibility for ensuring that you cover the right material is yours.

GRADING:

In-Class Participation: 20%

In-Class Quizzes: 40%

Final Project (20% oral; 20% written): 40%

100%

CREDITS AND GRADE OPTION: Students should register for 3 credits and with the (A-F) grade option.
## Tentative Schedule of Topics

<table>
<thead>
<tr>
<th>Week: Dates</th>
<th>Topics</th>
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<tbody>
<tr>
<td>1: 8/27, 8/29</td>
<td>Course introduction; Energy Levels and NMR Spectra (Ch. 1-3)</td>
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<tr>
<td>2: 9/3, 9/5</td>
<td>Energy Levels and NMR Spectra (Ch. 3)</td>
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<td>3: 9/10, 9/12</td>
<td>The Vector Model (Ch. 4)</td>
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<td>4: 9/17, 9/19</td>
<td>The Vector Model (Ch. 4); Fourier Transformation &amp; Data Processing (Ch. 5)</td>
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<td>5: 9/24, 9/26</td>
<td>Fourier Transformation &amp; Data Processing (Ch. 5); How the Spectrometer Works (Ch. 13)</td>
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<td>6: 10/1, 10/3</td>
<td>Product Operators (Ch. 7)*</td>
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<td>• *Ch. 6 is optional but strongly encouraged</td>
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<td></td>
<td>• Supplemental reading to be assigned</td>
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<tr>
<td>7: 10/8, 10/10</td>
<td>Product Operators</td>
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<tr>
<td>8: 10/15, 10/17</td>
<td>Product Operators</td>
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<td>9: 10/22, 10/24</td>
<td>Two-dimensional NMR (Ch. 8)</td>
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<td>10: 10/29, 10/31</td>
<td>Two-dimensional NMR; Relaxation and the NOE (Ch. 9)</td>
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<tr>
<td>11: 11/5, 11/7</td>
<td>Relaxation and the NOE (Ch. 9)</td>
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<td>12: 11/12, 11/14</td>
<td>Solid-state NMR spectroscopy</td>
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<td>• Reading to be assigned from other textbooks and current literature</td>
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<td>• Hamiltonian for SSNMR; interactions in the solid state; applications to organic and biological solids</td>
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<td>• Quadrupolar nuclei – terms in Hamiltonian, $^2$H NMR and dynamics measurements; heavier quadrupoles &amp; selected experiments, with applications to hard materials</td>
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<td>13: 11/19, 11/21</td>
<td>SSNMR (continued)</td>
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<tr>
<td>14: 11/26</td>
<td>SSNMR (continued) and/or Quiz</td>
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<td>15: 12/3, 12/5</td>
<td>Final Oral Presentations</td>
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<tr>
<td>16: 12/10, 12/12</td>
<td>Final Oral Presentations</td>
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Class Format and Grading for CHEM 751:

- Please read the assigned chapters before each class. My lectures closely follow the textbook, and most humans must see/hear/read the material on NMR spectroscopy more than once to understand it.

- As with nearly any chemistry course, we’ll reinforce the concepts covered in class with homework assignments. Homework will be assigned (roughly) every week, depending on the topic. One of the reasons for selecting this book is the online solutions; please take advantage of this resource.

- Tentatively, problem sets will be covered on Wednesdays. You should complete each problem set by the due date (before you come to class!). You will be assigned to present a problem (or part of the problem) on the board. Everyone is expected to participate in the discussion of the problems, related questions, etc.

- Tentatively, quizzes will be given at the beginning of the class period on Fridays. We will have a quiz (roughly) once a week (to follow the Problem Set). Each quiz will focus on the material in the most recently discussed Problem Set. It will not include the material that will be covered that day in the lecture, but everything (else) from the previous weeks is “fair game”.
  
  o Please be prompt, as time extensions and/or makeup quizzes will be allowed only in extremely unusual circumstances.

- Your “participation grade” will be based on your contributions to and conduct in class (as it relates to, e.g., problem-solving, group discussion, attendance).

Final Project:

- Your Final Project will focus on an NMR experiment (or set of related experiments) and an application of this experiment. You will present a talk (30-40 min, with an additional 5-10 minutes for questions), and you will also submit a written report that is based on the talk. The due date for the written portion is TBA (but likely during Finals Week).

- Possible topics for your Final Project:
  
  o A specific NMR experiment (e.g., HSQC-TOCSY, REDOR).
  
  o Characterization of a given sample using a set of techniques (e.g., dipolar recoupling experiments of amyloid)
  
  o An overview of related NMR techniques (e.g., solvent suppression methods).
  
  o An overview of NMR techniques used for a less common nucleus.
• The grade for your talk will be based on:
  o Content. Is the material accurate and appropriate? Is it clearly presented, based on the level of NMR we've covered in class?
  o Organization. Does your talk have a reasonable order of topics? Does it have the expected duration of 25-30 minutes? (Please note that talks that run for ≤20 minutes will be substantially penalized.)
  o Appearance and/or presentation (of the slides, not you).
  o Your oral communication skills.
  o Your answers to the questions that follow your talk.

• The written report is based on your talk. You can use many of the same figures, in addition to a narrative that should include:
  o Abstract (up to 250 words)
  o Introduction to provide background information, as well as the “rationale” behind doing the selected NMR experiment(s).
  o Description of the NMR experiment(s), including details such as pulse sequence(s), typical parameters (e.g., pulse widths, delay times), hardware requirements (especially probe type), and any special sample preparation conditions.
  o Description of the application(s). Describe the system of interest and how the selected NMR experiment answers key or critical questions. Show the spectrum (or spectra) that are obtained and how information is extracted. What are the results/discussion and conclusions?
  o General conclusions. Include a discussion of the strengths and drawbacks/challenges of the technique(s) and/or approach.
  o Figures that are legible and numbered sequentially. Figures should be embedded in the narrative. Figure captions are strongly recommended. Cite original sources, as necessary.
  o A typical report will be 15-20 pages long (including appropriately sized figures). Please do not use more than 25 pages to write your report, unless it is suitably brilliant and novel (e.g., your next manuscript for submission to an NMR journal).
  o The report should be double-spaced with a font size of 10 or 12. Use font size 10 or smaller for figure captions.
  o In the narrative itself, include citations to the literature and put the list of references at the end of your report, just as you would for a manuscript. The format is essentially up to you, but best is one that includes the complete author list (not just 1st author), full title of the article, journal name, volume, year, and pages (or at least first page). Databases and other online resources usually provide information on how you should cite them.