PRINCIPLES & APPLICATIONS
OF NMR SPECTROSCOPY

Chemistry 539
Tuesday 6-8:30 pm Campion Hall Room 204

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CASE STUDIES:       Menthol
                                2-Ethyl-1-indanone
                                Gramicidin-S

I.   THEORY

1) NMR Basics

2) Energy Levels and NMR Spectra

3) The Vector Model for NMR

4) Fourier Transform and Data Processing

5) The Quantum Mechanics of One Spin

6) Product Operators

7) Two-Dimensional NMR

8) Relaxation and the NOE

II. EXPERIMENTAL

1) Sample Preparation
   A. Solvent Selection
   B. Volume and Concentration Considerations

2) Spectrometer Setup
   A. Deuteration Lock
B. Probe Tuning
C. Adjusting Field Homogeneity (Shimming)

3) Data Acquisition
   A. Excitation Modes
   B. Acquisition Parameters
   C. Decoupling
   D. Inverse Detection

4) Data Processing
   A. Signal-to-Noise Enhancement
   B. Resolution Enhancement
   C. Phasing
   D. Baseline Corrections
   E. Transformations
   F. Peak Picking and Integration

5) Special 1-Dimensional NMR Experiments
   A. APT and DEPT
   B. NOE Difference Experiment
   C. Relaxation Time Measurements
   D. Solvent Suppression Techniques

6) Multi-dimensional NMR
   A. 2D Homonuclear
   B. 2D Heteronuclear
   C. 2D Inverse Detection

III. APPLICATIONS

1) Chemical Analysis
   A. Functional Group Analysis
   B. Stereo-chemical Discrimination

2) Molecular Dynamics and NMR
   A. Motional Effects on NMR Observables
   B. Chemical Exchange
   C. Ligand Binding
   D. Kinetics

3) Structure Analysis
   A. Solution Structure of Peptides and Proteins
   B. Bio-membrane Structure