Draft Syllabus last Revised: March 6, 2006

I. Introductory Information

A. Department Name:	Chemistry
B. Department Catalog Number:	CHEM 4 _ _
C. Course Title:	Spectroscopic Methods of Molecular Structure Determination
D. Semester Hour Credit:	3 hours
E. Clock Hours per Week:	3 hours lecture
F. Overlays:	None
G. Restrictions Upon Student Registration:	Prerequisite: CHEM 320; Pre- or Co-requisite CHEM 321.

II. Description of the Course

Focuses on the interpretation of spectral data. Theory of each spectroscopic method, sample preparation, instrumentation and applications of each method will also be discussed. Problems will be presented in class to demonstrate logical approaches to solving spectral problems. Student in-class problems will be used to generate open discussion. Spectral problems will be used to reinforce concepts and approaches to determining the structure of unknowns. Examples from both organic and inorganic chemistry will be used.

III. Exposition

A. Objectives:

Upon completion of the course, the student will be able to

1. explain the theory of the spectroscopic methods that are critical to determining the molecular structure of unknown compounds
2. explain the fundamentals of the spectroscopic instrumentation and sampling methods of the various spectroscopic techniques
3. identify which spectroscopic technique(s) is (are) appropriate for solving different problems and appreciate the advantages and disadvantages of each method toward solving structural determination problems
4. determine the structure of unknown compounds from spectral data
5. apply complimentary spectroscopic techniques toward solving complex problems
6. articulate the fundamental relationships between molecular structure and physical properties that are evident spectroscopically
7. interpret data obtained through state-of-the-art spectroscopic techniques

B. Activities and Requirements

1. In-class presentations and discussions will be used to present the theory of the various spectroscopic methods. Students will be assessed on III.A.1. through homework sets and exam questions.
2. In-class presentations, demonstrations, and laboratory demonstrations will be used to demonstrate the instrumentation and sampling methods for the various spectroscopic methods. Students will be assessed on III.A.2 through exam questions.

3. In-class group discussions and student-led discussions will be used to explore the advantages of the different techniques as we work through problems together in class. Students will be assessed on III.A.3. through their participation in class discussions and exam questions.
4. Students will solve spectral problems on homework, selected problems will be assigned to small groups for informal presentation to the class; in-class problems will also be assigned; spectral problems compose the majority of the in-class exams. In-class discussions will demonstrate logical strategies for solving spectral problems. Students will be assessed on III.A.4. through exam questions and their problem-solving sessions in class.
5. As their skills in interpreting spectroscopic data improve, the problems become more complex and more difficult. As the level of complexity increases, the students will need to utilize multiple sources of spectral data. Students will be assessed on III.A.5. individually (exams and homework problems) as well as in small groups (group problems and discussions led in class).
6. In-class presentations will be used to discuss the spectral evidence that supports our understanding of molecular structure and molecular processes. Students will be assessed on III.A.6. through homework problems and their responses during in-class discussions.
7. State-of-the-art methods of predicting spectral features and spectroscopic methods of determining subtleties in the molecular structures will be presented. Demonstrations of the available instrumentation will be used to supplement the lecture. Students will be assessed on III.A.7. through homework, in-class problems, and exam questions.

C. Major Units and Time Allotted

1. Infrared and Raman Spectroscopy (7 contact hours)
2. Nuclear Magnetic Resonance Spectroscopy (NMR) (17 contact hours)
3. UV-VIS Spectroscopy (5 contact hours)
4. Mass Spectrometry (11 contact hours)
5. Combined Spectral Problems (5 contact hours)

D. Materials and Bibliography

1. Suggested textbooks

a. Crews, Phillip; Jaime Rodriguez, and Marcel Jaspars, Organic Structure Analysis, Oxford University Press, NY, 1998.

b. Field, Leslie D.; S. Sternhell, and J. R. Kalman, Organic Structures for Spectra, 3rd Edition, John Wiley and Sons, 2002.

c. Pavia, Donald L., G. M.Lampman, and G. S. Kriz, Introduction to Spectroscopy: A Guide for Students of Organic Chemistry, 3rd Edition, Brooks-Cole, 2001.

d. Silverstein, R. M., G. C Bassler, and T. C. Morrill, Spectrometric Identification of Organic Compounds, Fourth Edition, John Wiley and Sons, NY, 1981.

e. Williams, D. H. and Ian Fleming, Spectroscopic Methods in Organic Chemistry, 5th Edition, McGraw-Hill, 1995.

f. Young, Paul, Practical Spectroscopy: The Rapid Interpretation of Spectral Data, 5 th Edition, Brooks-Cole, 2000.

2. Other Materials

NMR Simulator
Introduction to Spectroscopy
Organic Chemistry—Spectra of Compounds
IR Tutor
C-13 Calculator

3. Bibliographic Support

a. Books

i. Abraham, R. J., Introduction to NMR Spectroscopy, Wiley 1988.

ii. Akitt, J. W., NMR and Chemistry: An Introduction to Modern NMR Spectroscopy, Chapman and Hall, NY, 1992.

iii. Ault, Addison and Gerald.O. Dudek, NMR: An Introduction to Proton Nuclear Magnetic Resonance Spectroscopy, Holden-Day, San Francisco, CA, 1976.

iv. Bible, Roy Henderson, Interpretation of NMR Spectra: An Empirical Approach, Plenum Press, NY, 1965.

v. Brown, David W., Organic Spectroscopy, John Wiley and Sons, NY, 1988.

vi. Croasmun, William R. and Robert M. K. Carlson, Two Dimensional NMR Spectroscopy: Applications for Chemists and Biochemists, VCH, NY, 1994.

vii. Creswell, Clifford J. and Olaf Runquist, Spectral Analyses of Organic Compounds: An Introductory Programmed Text, Burgess Publishing Co., Minneapolis, MN, 1970.

viii. Crews, Phillip, Jaime Rodriguez, and Marcel Jaspars, Organic Structure Analysis, Oxford University Press, NY, 1998.

ix. Davis, R. and M. Frearson, Mass Spectrometry, John Wiley and Sons, NY, 1987.

x. Davis, R. and C.H.J. Wells, Spectral Problems in Organic Chemistry, Chapman and Hall, NY, 1984.

xi. Duddeck, Helmut and W.Dietrich, Structure Elucidation by Modern NMR: A Workbook, 3rd Edition, Springer-Verlag, NY, 1999.

xii. Feinstein, Karen, Guide to Spectroscopic Identification of Organic Compounds, CRC Press, Boca Raton, FL, 1995.

xiii. George, William O., and P. S. McIntyre, Infrared Spectroscopy, John Wiley and Sons, NY, 1987.

xiv. Gunther, H., NMR Spectroscopy: Basic Principles, Concepts, and Applications in Chemistry, Second Edition, Wiley, NY, 1995.

xv. Harrison, Alex G., Chemical Ionization Mass Spectrometry, CRC Press, Boca Raton, FL, 1992.

xvi. Hill, Roger and D.A.E. Rundell, The Interpretation of Infrared Spectra, A Programmed Introduction, Heyden, NY, 1975.

xvii. Kemp, William, NMR in Chemistry: A Multinuclear Introduction, Macmillan, Hampshire, 1986.

xviii. Laszlo, Pierre, NMR of Newly Accessible Nuclei, Academic Press, NY, 1983.

xix. Lee, Terrence A. Lee, A Beginner's Guide to Mass Spectral Interpretation, Wiley, NY 1998.

xx. McLafferty, Fred W. and Frantisek Turecek, Interpretation of Mass Spectra, Fourth Edition, University Science Books, Mill Valley, CA, 1993.

xxi. Martin, Gary E. and Andrew S. Zektzer, Two-Dimensional NMR Methods for Establishing Molecular Connectivity: A Chemist's Guide to Experiment Selection, Performance, and Interpretation, VCH Publishers, NY, 1988.

xxii. Roeges, Noel P.G., A Guide to the Complete Interpretation of Infrared Spectra of Organic Structures, Wiley, NY, 1994.

xxiii. Shraml, Jan and J. M. Bellama, Two Dimensional NMR Spectroscopy, Wiley, NY, 1988.

b. Relevant Journals available at Stevenson Library

Analytical Chemistry
Journal of the American Chemical Society
Journal of Chemical Education
Journal of Organic Chemistry
Journal of Inorganic Chemistry
Organometallics

IV. Standards

The grading criteria for this course will be according to current university grading policy. Grades will be based upon student demonstration of mastery of the objectives listed in section III.A., through the use of homework sets, exams, and problems assigned in class. Because a significant percentage of the class time will be devoted to the process of problem solving, attendance will be a component of the grading criteria.

V. Rationale and Impact

A. Why the Proposal is Necessary

This is a revision of an existing course; the revision of the syllabus and the proposal for changing the course number is necessary for fulfilling the ACS Curriculum Guidelines for program approval. Discussions of the theory of the methods will assume the necessary background provided by the physical chemistry courses, thus the need to assign a 4XX designation for the course. The name of the course is being changed from the original title (Spectroscopic Methods of Structure Determination) to one that more accurately describes the scope of the course and was the title originally proposed (Spectroscopic Methods of Molecular Structure Determination).

B. For whom Spectroscopic Methods is Specifically Designed

The course will serve as one of the required advanced courses having a physical chemistry prerequisite for the anticipated ACS-Approved B.S-Chemistry degree. The course would also count as an upper-level elective for students pursuing the Biology-Chemistry degree.

Spectroscopic Methods of Molecular Structure Determination provides students an opportunity to develop their problem-solving and critical thinking skills while learning a systematic approach to answering a fundamental question that is often encountered in chemistry: what is it? It is desirable that advanced students in chemistry and other sciences develop their skills in spectral interpretation, as these methods are becoming increasingly applicable to all the areas of science. The problem-solving skills that students develop in a spectral data interpretation course can be applied to many areas, such as synthesis, quality assurance, environmental analysis, structural determination of naturally-occurring compounds, identification of unknown compounds, and characterization of known compounds. Finally, many of the physical properties of compounds are evident in the spectral features, which helps students refine their understanding of the relationships between molecular structure, physical properties, and spectral properties of chemical compounds.

C. How Existing Academic Programs or Departments will be Affected by this Syllabus

In previous years, Spectroscopic Methods of Molecular Structure Determination has served as a Chemistry Elective for students majoring in Chemistry and Biology-Chemistry. Because of the restructuring of the B.S.-Chemistry curriculum, the course will become a required course for B.S.-Chemistry students. Because of the CHEM320/321 pre- or co-requisites, a large majority of students will be B.S.-Chemistry majors.

VI. Cost and Staff Analysis

No additional staff will be needed for the course. The three hours of faculty time are already accounted for in the normal rotation of Special Topics in the department. Since there is no laboratory being offered, there are no equipment or supply costs. Most materials for the course are accessible to the students in the Instrument Room, Stevenson Library, Pennsylvania State University Library, or the Internet. Some additional copies of the software will be desirable depending on the enrollment for the course.

VII. Date approved by the University President:

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Signature of the President Date