Spectrometric Identification of Organic Compounds

I. Course code: Class hours: 32 Credits: 2

II. Suitable specialty: Chemistry

III. Prerequisites: Fundamental knowledge of quantum chemistry, mass spectra and infrared techniques.

IV. Course goals:

This course will focus on the identification of unknown organic compounds using various spectroscopic techniques, such as mass spectra and infrared, with emphasis on NMR (Nuclear Magnetic Resonance). The theoretical aspects behind the various techniques will be briefly mentioned but not discussed in details.

V. Teaching method: lectures, discussion, paper analysis

VI. Contents:

1. Proton magnetic resonance spectroscopy 2 class hours
   - 1.1 Introduction
   - 1.2 Theory
   - 1.3 Instrumentation and sample handling
2. Chemical shift 2 class hours
3. Spin coupling, multiplets, spin systems 4 class hours
4. Exchangeable protons 4 class hours
5. Coupling of protons to other nuclei 4 class hours
   - 5.1 Coupling of protons to ^{19}F
   - 5.2 Coupling of protons to ^{31}P
   - 5.3 Coupling of protons to ^{13}C
6. Chemical shift equivalence 4 class hours
   - 6.1 Determination of chemical shift equivalence by interchange through symmetry operations
   - 6.2 Determination of chemical shift equivalence by Tagging
   - 6.3 Chemical shift equivalence by rapid interconversion of structures
7. Carbon-13 NMR spectrometry 4 class hours
   - 7.1 Introduction

7.2 Theory

7.3 Interpretation of simple ^{13}C spectra

8. Correlation NMR spectrometry 6 class hours

8.1 Theory

8.2 Correlation spectrometry

9. Infrared and Mass spectrometry 2 class hours

VII. Examination and grading:

The score uses a hundred-mark system.

Total Score 100%: Classroom performance 10%, take home exam 50%, in class exam 40%

VIII. Reference books

- NMR – From Spectra to Structures An Experimental approach
  Second edition (2007) Springler-Verlag
  Terence N. Mitchell, Burkhard Costisella
- Spectrometric Identification of Organic Compounds
  John Wiley & Sins, inc., sixth edition (or later).
  Robert M. Silverstein and Francis X. Webster
- Organic Structural Spectrocopy
  Prentice Hall inc., 1998
  Joseph B. Lambert, Herbert F. Shurvel, David A. Lightner, R. Graham Cooks
- NMR Spectroscopy, Basic principles, concepts, and applications in chemistry", second edition, John Wiley & Sins, inc., 1995.
  Harald Günther
- Modern NMR Spectroscopy, A Guide for Chemists,
  Oxford University Press, 1987
  Jeremy K.M. Sanders, Brian K. Hunter
- Organic Structure Analysis",
  Oxford University Press, 1998.
  Phillip Crews, Jaime Rofriguez, Marcel Jaspars
- Organic Structures from spectra
  Wiley (2008)
  L.D.Field, S.Sternhell and J.R.Kalman.

IX. Syllabus writer: Nan Wang

有机光谱分析

一． Course code: 课内学时: 32 学分: 2

二．适用专业：化学

三．选课基础：量子化学基础、质谱及红外光谱相关基础知识

四．教学目的：

本课程探讨使用各种光谱技术手段，例如质谱和红外等方法鉴定分析未知的有机化合物，其中将对核磁方法进行着重阐述。各种技术手段背后的基本原理将予以简要阐述，但不会过多的涉及细节方面的知识。

五．授课方式：

课堂授课、讨论，文献分析

六．教学主要内容：

1. 质子核磁共振谱（绪论） 2 学时

1.1 引言

1.2 理论

1.3 仪器和样品处理

2. 化学位移 2 学时

3. 自旋偶合、多重峰、自旋体系 4 学时

4. 可交换质子 4 学时

5. 质子对其他重要核的偶合 4 学时

5.1 质子对 ^{19}F 的偶合

5.2 质子对 ^{31}P 的偶合

5.3 质子对 ^{13}C 的偶合

6. 化学位移等价 4 学时

6.1 通过对称操作的互换检测化学位移等价

6.2 通过标记确定化学位移等价

6.3 结构快速互变引起的化学位移等价

7. 核磁共振碳 13 谱 4 学时

7.1 引言

7.2 理论

7.3 简单的碳 13 谱解析

8　核磁共振相关谱　6 学时

8.1 理论

8.2 相关谱

9　红外和质谱　2 学时

七．考核与成绩评定

成绩以百分制衡量。

评定依据：课堂表现 10%，课后考试 50%，课堂考试 40%

八．参考书

NMR – From Spectra to Structures An Experimental approach
Second edition (2007) Springler-Verlag
Terence N. Mitchell,　Burkhard Costisella

Spectrometric Identification of Organic Compounds
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Wiley (2008)
L.D.Field, S.Sternhell and J.R.Kalman.

九．大纲撰写人：王楠