波谱分析

一、课程编码：1000009

课内学时：32　学分：2

二、适用专业：化学工程与工艺、制药工程、应用化学、材料化学、有机化学

三、先修课程：有机化学

四、教学目的：

波谱分析是综合应用质谱（MS）、核磁共振波谱（NMR)、红外光谱(IR)和紫外光谱(UV)四大现代物理手段，研究有机化合物结构的一门科学，也是现代有机化合物结构鉴定的重要手段之一。本课程将使学生深入了解四大光谱，特别是质谱（MS）和核磁共振波谱（NMR）的原理及其在有机化合物结构鉴定中的作用。本课程的目的是培养学生综合应用有机波谱学知识分析鉴定有机化合物结构的能力。课程的重点是波谱的特征数据和化合物结构的关系，及其基本解析方法。

五、教学方式

以课堂讲授为主，辅以课堂讨论和演示

六、教学内容

1. 质谱　6 学时

1.1　质谱的基本知识

1.2　有机质谱中的裂解反应和裂解规律

1.3　常见各类化合物的质谱特点

1.4　分子量和分子式的确定

1.5　质谱图谱解析和分子结构确定

2. 红外吸收光谱　6 学时

2.1　红外吸收光谱的基本原理

2.2　红外光谱与分子结构的关系

2.3　各类化合物的红外光谱特征

2.4　红外光谱的解析

3. 核磁共振波谱　12 学时

3.1　核磁共振氢谱

3.2　核磁共振碳谱

3.3　二维核磁共振波谱

3.4　核磁共振波谱综合解析

4. 四谱综合解析　4 学时

4.1　综合分析的一般步骤

4.2　综合解析实例

5. 课堂讨论　4 学时

七、考核与成绩评定

成绩以百分制衡量。

成绩评定依据：课堂成绩 30%，考试 70%。

八、教材及参考书：

[1] 王鹏，冯金生，金韶华，徐志斌.有机波谱，国防工业出版社，2012.

[2] Robert M. Silverstein, Francis X. Webster，David J. Kiemle. Spectrometric identification of organic compounds (seventh edition), John Wiley &Sons,Inc,2005.

[3] 宁永成. 有机化合物结构鉴定与有机波谱学(第三版)，科学出版社, 2014.

十、大纲撰写人：冯金生，徐志斌，温鸿亮

Spectroscopic Analysis

I. Course code: 100009 Class hours: 32 Credits: 2

II. Suitable specialty: Chemistry Engineering & Technical Process, Pharmaceutical engineering, Applied Chemistry, Material Chemistry, Organic Chemistry

III. Prerequisites: Organic Chemistry

IV. Course goals:

Nowadays spectroscopy is being used as the most popular technique for structure determination and analysis. Thus, the knowledge of spectroscopy has become necessary for all the students of chemistry. This course will concentrate upon the mostly used techniques in organic structure determination: nuclear magnetic resonance (NMR), infrared (IR), ultraviolet-visible (UV-Vis) and mass spectrometry (MS). The main purpose of this course is to provide an introduction to organic spectroscopic analysis, leading to an appreciation of the information available from each form of spectroscopy and an ability to use spectroscopic information in the identification of organic compounds.

V. Teaching method:

Classroom lectures, classroom discuss

VI. Contents of Teaching:

1. Mass spectrometry 6 class hours

1.1 Theory

1.2 Fragmentation processes

1.3 Mass spectra of chemical classes

1.4 Mass spectra analysis and application

2. Infrared spectrometry 6 class hours

2.1 Theory

2.2 Fundamental vibrations and affecting factors

2.3 Characteristic absorptions in common classes of compounds

2.4 Interpretation and application of IR

3. Nuclear magnetic resonance spectroscopy 12 class hours

3.1 Introduction

3.2 Proton nuclear magnetic resonance spectroscopy

3.3 Carbon-13 NMR spectrometry

3.4 Correlation NMR spectrometry & 2-D NMR

3.5 Comprehensive analysis of the NMR spectra

4. Structure elucidation using all of the spectroscopic information available 4 class hours

4.1 General procedure

4.2 Exercises and discusses

5. Classroom Discussion 4 class hours

VII. Examination and grading:

The score uses a hundred-mark system.

Total Score 100%: Classroom performance 30%, Final Written Examination70%.

VIII. Textbook and reference:

[1] Peng Wang, Jinsheng Feng, Shaohua Jin, Zhibin XU. Organic spectroscopy, National Defense Industry Press, 2012 (Chinese).
[2] Robert M. Silverstein, Francis X. Webster， David J. Kiemle. Spectrometric identification of organic compounds (seventh edition), John Wiley & Sons, Inc, 2005 (English).
[3] Yongcheng Ning. Structural identification of organic compounds and organic spectroscopy (3rd edition), Science Press (P. R. China), 2014 (Chiense).
IX. Syllabus writer: Jinsheng Feng, Zhibin Xu, Hongliang Wen.