UNIVERSITI TEKNOLOGI MARA

CHM580: SPECTROCHEMICAL METHODS OF ANALYSIS

Course Name (English)	SPECTROCHEMICAL METHODS OF ANALYSIS APPROVED
Course Code	CHM580
MQF Credit	3
Course Description	This course will engage students cognitively and scientifically in areas of spectroscopic methods of analysis. Students will be exposed to definitions, concepts, and principles of spectroscopy. The students will also be expected to perform scientific investigations via laboratory exercises qualitatively and quantitatively. The outcomes shall be assessed through a variety of tools which include the final examination, tests, quizzes, laboratory reports and assignments.
Transferable Skills	Upon completion of this course, students should be able to: 1. To understand the concepts and theories in atomic and molecular spectroscopic instrumentation. 2. To conduct spectroscopic instrumentation techniques in qualitative and quantitative analysis.
Teaching Methodologies	Lectures, Lab Work, Discussion
CLO	CLO1 Explain at least four concepts and theories in atomic and molecular spectroscopic instrumentations: atomic absorption, atomic emission, UV-Vis, fluorescence, infrared, Raman, mass and nuclear magnetic resonance. CLO2 Apply spectroscopic instrumentation techniques to obtain qualitative and quantitative information about the composition and structure of matter. CLO3 Conduct scientific investigations in areas of spectroscopic methods of analysis. CLO4 Communicate in writing the scientific investigations in areas of spectroscopy.
Pre-Requisite Courses	No course recommendations

Topics
1. Introduction to Spectrometric Methods 1.1) 1.1 General Properties of Electromagnetic Radiation 1.2) 1.1.1 Wave and Quantum-Mechanical Properties of Electromagnetic Radiation 1.3) 1.1.2 The Electromagnetic Spectrum 1.4) 1.1.3 Energy States of Chemical Species 1.5) 1.1.4 Interaction of Radiation and Matter such as absorption, emission, luminescence and scattering 1.6) 1.2 Quantitative Aspects of Spectrochemical Measurements 1.7) 1.2.1 Transmittance 1.8) 1.2.2 Absorbance 1.9) 1.2.3 Beer's Law
2. Introduction of Optical Instruments 2.1) 2.1 General Designs of Optical Instruments 2.2) 2.2 Sources of Radiation (continuous, line and laser), wavelengths Selectors (grating monochromators), sample containers, and transducers (Photomultiplier Tubes, Photodiode Arrays and thermocouples)
3. Atomic Absorption (AA) Spectroscopy 3.1) 3.1 Fundamental Principles 3.2) 3.1.1 Energy Level diagrams 3.3) 3.1.2 Atomic Emission Spectra 3.4) 3.1.3 Atomic Absorption Spectra 3.5) 3.1.4 Atomic Line Widths 3.6) 3.1.4.1 Doppler Broadening 3.7) 3.1.4.2 Pressure Broadening

3.8) 3.1.5 The Effect of Temperature on Atomic Spectra
3.9) 3.2 Sample Atomization techniques
3.10) 3.2.1 Flame Atomization
3.11) 3.2.1.1 Types of Flame
3.12) 3.2.1.2 Flame Structure
3.13) 3.2.1.3 Flame Atomizers
3.14) 3.2.1.4 Performance Characteristics of Flame Atomizers
3.15) 3.2.2 Electrothermal Atomization
3.16) 3.2.2.1 Electrothermal Atomizers
3.17) 3.2.2.2 Output Signals
3.18) 3.2.2.3 Performance Characteristics of Electrothermal Atomizers
3.19) 3.2.2.4 Analysis of Solids
3.20) 3.3 Atomic Absorption Instrumentation
3.21) 3.3.1 Sample Introduction Methods
3.22) 3.3.2 Introduction of Solution Samples
3.23) 3.3.2.1 Nebulization
3.24) 3.3.2.2 Electrothermal Vaporizer
3.25) 3.3.3 Introduction of Solid Samples; Direct-sample Insertion, Electrothermal
3.26) Vaporizer, Laser ablation
3.27) 3.3.3.1 Electrothermal Vaporizer
3.28) 3.3.4 Radiation Sources
3.29) 3.3.4.1 Hollow Cathode Lamps
3.30) 3.3.4.2 Electrodeless Discharge Lamps
3.31) 3.3.5 Source Modulation
3.32) 3.4 Interferences
3.33) 3.4.1 Spectral Interferences
3.34) 3.4.2 Chemical Interferences
3.35) 3.4.2.1 Formation of Low Volatility Compounds
3.36) 3.4.2.2 Dissociation Equilibria
3.37) 3.4.2.3 Ionization Equilibria
3.38) 3.5 Sample Preparation (Acid digestion/microwave digestion)
3.39) 3.6 Quantitative Analysis; Standard Calibration Curve and Standard Addition Method.
3.40) 3.7 Application of AAS, Detection Limits and Accuracy

4. Atomic Emission (AE) Spectrometry
4.1) 4.1 Fundamental Principles
4.2) 4.2 AES based on Inductively Coupled Plasma (ICP) Source
4.3) 4.3 Application of ICP-OES; Sample Preparation, Elements Determined, Line Selection, Calibration Curves, Interferences and Detection limits.

5. Ultraviolet/Visible Molecular Absorption Spectrometry
5.1) 5.1 Measurement of Transmittance and Absorbance
5.2) 5.2 Beer's Law
5.3) 5.3 Limitations to Beer's Law; Real, Chemical and Instrumental Deviations.
5.4) 5.4 Instrumentation
5.5) 5.4.1 Radiation Sources; Deuterium and Hydrogen Lamps, Tungsten Halogen Lamps
5.6) 5.4.2 Sample Containers
5.7) 5.4.3 Types of Instrument; Single-Beam and Double-Beam Instruments
5.8) 5.5 Absorbing species; Organic Compounds, Inorganic Species and Charge Transfer Complexes.
5.9) 5.6 Quantitative Applications

6. Molecular Luminescence Spectrometry
6.1) 6.1 Theory of Fluorescence and phosphorescence
6.2) 6.1.1 Excited States Producing Fluorescence and phosphorescence
6.3) 6.1.2 Electron Spin
6.4) 6.1.3 Singlet and Triplet Excited States
6.5) 6.2 Energy-level diagrams
6.6) 6.3 Variables affecting fluorescence
6.7) 6.3.1 Quantum yield
6.8) 6.3.2 Transition types in fluorescence
6.9) 6.3.3 Fluorescence and structure
6.10) 6.3.4 Effect of structural rigidity
6.11) 6.3.5 Temperature effects
6.12) 6.3.6 Effect of concentration on fluorescence Intensity
6.13) 6.4 Components of spectrofluorometers; radiation sources, monochromators, transducers, cell and cell compartment
6.14) 6.5 Applications of fluorescence spectrometry

7. Infrared Spectrometry
7.1) 7.1 Theory of IR absorption
7.2) 7.2 IR Instrumentation; dispersive and FTIR
7.3) 7.3 Application: Mid-IR absorption spectrometry
7.4) 7.4 Sample handling
7.5) 7.5 Correlation charts and tables
7.6) 7.6 Interpretation of IR spectra of simple organic compounds (alkanes, alkenes, alkynes, alcohols, aldehydes, ketones, carboxylic acids, esters, ethers, aromatic hydrocarbons, amines and amides).

8. Raman spectroscopy
8.1) 8.1 Theory of Raman spectroscopy
8.2) 8.2 Energy-level diagrams
8.3) 8.3 Instrumentation
8.4) 8.4 Applications

9. Nuclear Magnetic Resonance (NMR) Spectroscopy
9.1) 9.1 Theory of NMR
9.2) 9.1.1 Quantum Description of NMR
9.3) 9.1.2 Energy Levels in a Magnetic Field
9.4) 9.1.3 Precession of Nuclei in a Field
9.5) 9.1.4 Origin of signal in FTNMR
9.6) 9.2 Instrumentation; CW and FT NMR
9.7) 9.2.1 Components of FT NMR spectrometers
9.8) 9.2.1.1 Magnets: locking the Magnetic Field, Shimming, Sample Spinning
9.9) 9.2.1.2 The sample probe
9.10) 9.2.1.3 Detector and Data-processing System
9.11) 9.2.2 Sample Handling
9.12) 9.3 Chemical Shift and its Measurement
9.13) 9.4 Factors influencing Chemical Shift
9.14) 9.5 Proton NMR Spectroscopy
9.15) 9.5.1 Solvents Used in NMR
9.16) 9.5.2 Integrals in Proton NMR Spectra
9.17) 9.5.3 Spin-Spin Coupling/Spin-Spin Splitting
9.18) 9.5.4 n+1 Rule
9.19) 9.5.5 Correlation Charts and Tables for Proton NMR
9.20) 9.5.6 Interpretation of Proton NMR Spectra of Simple Organic Compounds
9.21) 9.6 Carbon-13 NMR Spectroscopy
9.22) 9.6.1 Natural Abundance C-13 NMR Spectra
9.23) 9.6.2 Proton Decoupling
9.24) 9.6.2 Structural Applications of C-13 NMR
9.25) 9.6.3 Correlation Data and Tables for C-13 NMR Spectra
9.26) 9.6.4 Interpretation of C-13 NMR spectra
9.27) 9.7 Structure Elucidation of Simple Organic Compounds from IR and NMR spectra

10. Molecular Mass Spectroscopy
10.1) 10.1 Basic Principles
10.2) 10.2 Instrumentation
10.3) 10.2.1 Types of Ionization Sources; Gas phase (CI, EI, ESI and FAB)
10.4) 10.2.2 Types of Mass Analyzers; Magnetic Sector, Quadrupole, and Time-of-Flight
10.5) 10.3 Mass Spectra (EI and ESI)
10.6) 10.3.1 Isotope Abundances
10.7) 10.3.2 The Molecular Ion, Base Peak and Isotope Ratio (Chlorine or Bromine)
10.8) 10.3.3 Fragment ions (refers to EI)
10.9) 10.4 Applications of Molecular Mass Spectrometry (EI);
10.10) 10.4.1 Structural Analysis and Fragmentation Patterns: alkanes, alkenes, alkynes, aldehydes, ketones, alcohols.
10.11) 10.4.2 Mc Lafferty Rearrangement
10.12) 10.4.3 Molecular Mass Determination

Assessment Breakdown	%
Continuous Assessment	60.00%
Final Assessment	40.00%

Details of Continuous Assessment

Assessment Type	Assessment Description	% of Total Mark	CLO
Assignment	assess selected topics in chapter 5, 6,7, 8, 9, 10	20%	CLO2
Practical	Lab skill	5%	CLO3
Test	Test 1 covers chap 1,2,3 and 4	20%	CLO1
Written Report	written report	15%	CLO4

Reading List

Recommended Text

- **Douglas A. Skoog,F. James Holler,Stanley R. Crouch 2007, *Principles of Instrumental Analysis*, Brooks/Cole Publishing Company [ISBN: 9780495012016]**

Reference Book Resources

- **Donald Pavia,Gary Lampman,George Kriz,James Vyvyan 2008, *Introduction to Spectroscopy*, Cengage Learning [ISBN: 9780495114789]**
- **Daniel C. Harris 2010, *Quantitative Chemical Analysis*, Macmillan [ISBN: 9781429218153]**
- **Francis Rouessac,Annick Rouessac 2007, *Chemical analysis*, Wiley [ISBN: 9780470859025]**
- **Douglas A. Skoog 2000, *Analytical Chemistry*, Brooks/Cole Publishing Company [ISBN: 0030202930]**

Article/Paper List: This Course does not have any article/paper resources

Other References: This Course does not have any other resources