Freie Universität Berlin

Institute of Chemistry and Biochemistry

Course description

Course Title
Modern Methods in Mass Spectroscopy / Métodos Modernos em Espectroscopia de Massa

Type/Attendance Time	Credit points (ECTS)	Type of Examination
Lecture: 2 hours per week	3	oral exam

Recommended Prerequisites: none

Content

1. Introduction: Why Mass Spectrometry, Historical Remarks, Information Content of a Mass Spectrum, General Scheme of a Mass Spectrometer, Vacuum Technology, Terms and Units
2. Ionization Methods: Electron Ionization (EI), Closed-Shell Quasi-Molecular Ions: Chemical Ionization (CI), Fast-Atom-Bombardment (FAB), Matrix-Assisted Laser Desorption/Ionization (MALDI), Electrospray Ionization (ESI)
3. Fragmentations in the EI Ion Source: Open- and Closed-Shell Ions, Preferred Decomposition Reactions of Cation Radicals, Thermal Decomposition in the Inlet System, Ion/Dipole Complexes, Distonic Ions
4. Analyzers and Detectors: Sector-Field Instruments, Linear Quadrupols and Quadrupole Ion Traps, Time-of-Flight Instruments, Fourier-Transform-Ion-Cyclotron-Resonance Mass Spectrometers
5. Ion Energetics in High Vacuum: Vertical and Adiabatic Ionization, Franck-Condon Principle, Stable - Metastable - Unstable, Quasi-Equilibrium Theory (QET), Temperature Dilemma: Non-Boltzmann Distribution of Inner Energies, Environmental Effects: Absolute Acidity - Gas-Phase Proton Affinities, Nucleophilic Substitutions in the Gas Phase
6. Isotopes and Isotope Effects: Isotope Patterns and Elemental Composition, Kinetic Isotope Effects
7. Hyphenated Methods (GC-MS, LC-MS): Basics of Chromatography, GC-MS Coupling, LC-MS Coupling
8. Tandem Mass Spectrometry and Gas-Phase Chemistry: Mass Selection, Metastable Ions and Collisional Activation, Bimolecular Reactions, MS for the Analysis of Dendritic Effects, Peptide Sequences from MS- and MS/MS Experiments, Radiative Processes: IRMPD and BIRD, Thermochemical Data: Ways out of the Temperature Dilemma, The Best-Fit Model of Alkali-Crownether Binding
9. Demonstration of Instruments: EI-Sector-Field Instrument, ESI-FTICR, Tandem-MS, GC-MS and LC-MS
10. Excercises

Conteúdo

1. Introdução
2. Métodos de ionização;
3. Fragmentações na fonte íon EI
4. Analisadores e detectores;
5. Energética de íon em alto vácuo;
6. Isótopos e efeito isótopo;
7. Métodos hifenizados (GC-MS, LC-MS);
8. Espectroscopia de massa Tandem e química em fase gasosa;
9. Demonstração de instrumentos;
10. Exercícios.