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Chapter 1 : BioZone Mass Spectrometry | BioZone

In modern times, mass spectrometry (MS) is widely used in the characterization of proteins at the intact (native) and peptide levels, as well as in the analysis of enzymatically generated protein fragments, in conjunction with an expanding range of compatible chromatographic separation techniques.

By Mike Grayson This year, we celebrated the centenary of J. Thomson was most definitely a visionary, but the chemical community was not quite ready to embrace the positive ray analyzer, what we now know as the mass spectrometer. Of course, much groundwork had been done by a variety of researchers prior to , providing Thomson with a foundation to base his research on. The Gas Discharge Experiment The origins of mass spectrometry began with the earliest gas discharge experiments. These were conducted in a partially evacuated glass envelope in which electrodes were inserted. At an appropriate gas pressure and voltage across the electrodes, a variety of glowing light phenomena were observed. While frequently used as an entertaining display of the curious properties of electricity, a number of serious researchers were intent on better understanding the various phenomena. Originally, only qualitative observations could be recorded; how the glow in the tube changed with pressure, nature of the gas, and magnitude of the voltage. Philosophical Transactions of the Royal Society of London, 4 Thomson and the properties of the electron One of the earliest scientific puzzles posed by the gas discharge experiment was whether or not charged particles were involved, or only light was produced. Kanalstrahlen in the gas discharge experiment Many of the same researchers who investigated cathode rays also turned to the study of kanalstrahlen, or positively charged particles, produced in the gas discharge experiment. At first Goldstein thought they were unaffected by magnetic fields. Later Wien and Thomson showed that kanalstrahlen could be deflected if the magnetic field was strong enough. A Apparatus Goldstein used to observe kanalstrahlen, rays of positive electricity, circa London, A , 89, The glass volume in the center is where the gas discharge took place. He began to develop a new mass analyzer which he would improve over several decades. He still relied on the gas discharge experiment to produce ions for analysis, but was able to obtain much better mass spectra. Exploring the elements for isotopes Beginning in the early s, Aston began a life-long investigation of the elements and their isotopes, determining their precise mass and relative abundance. During his career, he published almost 70 journal articles and several books on the subject. While others in Europe and America made some contributions, Aston essentially owned the field. Mass Spec Pioneer Alfred O. Nier, perhaps more than any other physicist, helped to spread the application of mass spectrometry in many different scientific fields. With a strong background in electrical engineering and excellent experimental skills, he specialized in creating inexpensive, reliable instruments suitable for specific applications isotope ratio analysis, leak detection, process control, general analytical, upper atmosphere analysis, planetary atmosphere analysis, respiratory gas analysis. He gave away his instruments and expertise to colleagues both inside and outside the physics and University of Minnesota communities. The double focusing instrument provided higher resolving and improved mass measurement accuracy for the study of the elements. Commercial variations of this mass analyzer design were successfully marketed up until the s. Dempster, working at the University of Chicago, built a positive ray analyzer similar to that of Thomson and he too decided that a new mass analyzer was needed. They developed more powerful instruments, refined the accuracy of measurements of the relative abundance and masses of the elements and their isotopes, and broadened the application of mass spectrometry to areas outside the realm of physics.

Chapter 2 : Modern mass spectrometry | Feature | Education in Chemistry

Mass spectrometry (MS) relies, among other things, on two fundamental criteria. The atom or compound of interest must be ionised to generate charged species, and these are then mass analysed to determine their mass-to-charge (m/z) ratio.

Advances in mass spectrometry MS technology over the past 30 years have pushed this technique into the hands of biologists and biochemists, and led to a host of new applications. In Short The development of soft ionisation techniques has meant MS can be used to analyse large biological molecules Protein analysis, the quality control of biofuels, and forensics all benefit from advances in MS technology Mass spectrometry MS relies, among other things, on two fundamental criteria. Further, MS is increasingly finding application in solving biological problems. The ions formed are then accelerated by an electric field and pass through a mass analyser. The following relationship applies: Further, the molecules do not have to be in the gas phase prior to ionisation. Thus thermally unstable molecules of biological relevance could now be analysed using MS. The resulting solution is then spotted onto a sample plate and irradiated with a laser. Typically, a laser with a wavelength in the uv region of the electromagnetic spectrum is used. The matrix absorbs at or near the laser wavelength, which causes the matrix molecules to sublime from the surface. Analyte molecules are carried with them and ionisation takes place in the gas phase immediately above the sample plate. The ions are then sampled into the mass analyser. The solution is passed through a metal capillary to which a high voltage, usually between kV for positive ESI, is applied Fig 3. A counter electrode is held at 0 V, causing a strong electrical field to be created. Consequently, the solution comes out of the capillary as small droplets, which become smaller as solvent molecules evaporate, eventually leaving the isolated ions to enter the mass spectrometer. Conversely, negative ESI can be performed where a proton is abstracted from an acidic group on the analyte by using negative voltages. This leads to a range of species existing in solution, differentiated by the number of protons attached to the molecule. The annotations Fig 4 show the number of protons associated with each peak. Deconvolution of the spectrum allows the molecular weight of the protein analysed to be determined. Reproduced with permission from the American Association for the Advancement of Science. Fenn was awarded the Nobel Prize for chemistry in in recognition of the immense impact that ESI had on the scientific world. He demonstrated that large molecules in excess of , Da could be ionised using his new technique. The analyte need not be dissolved in a matrix as in MALDI , thus negating the need for sample preparation. Thinkstock DESI could find its way to airport check-ins for high-throughput analyses of drugs and explosives In DESI, the same solvents as used for conventional ESI are electrosprayed onto the surface containing the analyte of interest. Upon contact with the surface, the droplets transfer energy, causing the molecules to desorb and become ionised. The same types of ions as conventional ESI, including multiply-charged species, can be observed. An advantage of DESI is that the removal of the sample preparation step makes the technique suitable for high-throughput analyses, such as checking luggage for traces of drugs and explosives at airports. Mass analyser technology has developed, leading to faster and more selective instruments. As such analysts can detect more compounds and have greater confidence that they are identifying them correctly. This ensures that the spectra recorded are not composites of more than one compound. This is especially important for modern mass spectrometric analyses where complex matrices of potentially thousands of compounds are encountered. Bodily fluids in biological MS and mixtures of hydrocarbons in biofuel analysis are two examples. The chemistry of the analyte of interest determines which approach is used, but both methods can easily be coupled to MS. The instrument consists of a column to which a stationary phase is bonded. The gaseous or liquid mobile phase containing the sample then passes over it. Thus, separation is achieved. Examples include metabolomics, where endogenous metabolites are profiled, glycomics, which involves identifying the entire complement of sugars, and proteomics, the analysis of proteins in biological systems. A typical proteomics experiment involves analysing the proteins present in a diseased tissue for example, the cells of a cancerous organ and comparing the results with those from a healthy, control sample. The increased or decreased expression of certain proteins can be used as biomarkers

for the disease in question. Mass spectrometry is ideally suited to this task, owing to its low limit of detection. The sequence information in a proteomics experiment can be derived from either the protein itself or its constituent peptides. Either approach will produce fragment ions that are related to the sequence of amino acids constituting the peptide or protein. The sequence can then be deduced from first principles or by reference to a database to identify the protein. MS for a green future Source: The mass spectrometer is interfaced to a gas chromatograph, essential owing to the complex nature of petrochemical matrices, and can be used to monitor both the FAMEs fatty acid methyl esters, the constituents of biodiesel in the sample as well as any impurities and degradation products that could damage or clog the engine. The older technology of EI is particularly useful, producing diagnostic fragmentation patterns that can be compared against databases to identify the compounds in the biodiesel. By using the intensities of the signals produced by the compounds in the sample and comparing them to that generated for an internal standard, an accurate estimate of each compound can be made using GC-MS. This is particularly important because UK legislation requires all diesel to be 5 per cent biodiesel by A common imaging MS experiment involves the detection of a biologically relevant compound in a tissue. In an example, thin slices of rat brain were made after the drug olanzapine had been administered. The images were obtained by taking spectra across the whole tissue section, thus producing a mass spectrum at each x, y coordinate. By converting the ion intensity to colour at each point, the distribution of olanzapine was shown to have decreased in the brain and spinal cord after six hours compared to after two hours. This showed that the drug was cleared from the central nervous system in this time period. MS is increasingly finding application in the understanding of pharmaceutical drug metabolism, in toxicological screening for drugs of abuse in athletes, in the measurement of heavy metals in environmental samples and many other areas. It is anticipated that increased usage of existing MS technology, coupled with new instrumental developments, will see the use of the technique become even more common in the future. John Wiley and Sons, Van Gerpen and J.

Chapter 3 : modern mass spectrometry | Download eBook pdf, epub, tuebl, mobi

Ion mobility spectrometry-mass spectrometry (IMS/MS or IMMS) is a technique where ions are first separated by drift time through some neutral gas under an applied electrical potential gradient before being introduced into a mass spectrometer.

December 19, Lewis; both have profound connections to the first. His student, Aston, who built more mass spectrometers, expanded the discipline, identified of the naturally occurring isotopes and became the first Nobel Laureate in Chemistry in the area. Five Nobel Prizes have been awarded to MS pioneers. Mass spectrometry is a way to measure the mass of ions â€" electrically charged species, derived from atoms or molecules. The words were prophetic. Today, there is no single area of experimental science where mass spectroscopy is not being used. There is no university or research institution in the developed world without a mass spectrometer; this may even be said about India. The technique is used to explore the chemical constitution of molecules from this planet and beyond, e. It is used to understand the fundamental atomic and molecular processes and at the same time those of immediate relevance to events within cells. As a technique, it helps to control processes in chemical and biological industries, diagnose diseases, discover new drugs, protect the environment and explore mysteries of nature. In years, it has been used to separate much of the uranium used to make the Little Boy the bomb that was dropped onto Hiroshima in , led to understanding of thousands of chemical reactions, to the discovery of new molecules, to the resolution of protein structures, to solve crimes and to provide answers to complex questions of nature. Mass spectrometers require a way to produce ions â€" e. In each of these areas forming ions, analysing their mass, detecting them innovations have led to multiple mass spectrometric techniques. The most important developments have happened in ion formation. Years ago, it was necessary to evaporate a sample to generate vapours and bombard these with a stream of electrons in order to make ions, a process which required vacuum. This was possible only with simple molecules which can be evaporated, generally by heating. Today it is possible to measure the mass spectrum of complex proteins, extremely fragile molecular assemblies and even intact cells, none of which evaporate normally. It is now possible to measure mass spectra of ultra small volumes, as small as a single human cell. It is possible to understand the spectrum of molecules from the surface of a rose while the plant is alive. It has been demonstrated that they can help in diagnosis during complex surgeries within the operating theatre. Ions are enjoying a considerable following these days. The mass spectrometry community is probably the largest group of scientists working around a single tool. However, despite this large following, it is surprising that mass spectrometry is being removed gradually from our science curriculum. Mass spectrometry concerns ion chemistry and physics with an emphasis on scientific instrumentation. However, in the past several years, paralleling the growth of applications of the method, spectrometers have become black boxes for the vast majority. Sadly, in the process, Thomson is forgotten. Appreciation of instrumentation should be brought back to the curriculum. We must note that Thomson, after considerable work in theoretical physics, moved to experiments. The Nobel committee over many years has demonstrated its appreciation for scientific instrumentation; this is a lesson we in India cannot afford to discard.

Chapter 4 : Department of Chemistry | NC State University

1 Modern Mass Spectrometry MacMillan Group Meeting Sandra Lee Key References: E. Uggerud, S. Petrie, D. K. Bohme, F. Turecek, D. SchrÃ¶der, H. Schwarz, D.

History of mass spectrometry Replica of J. Goldstein called these positively charged anode rays "Kanalstrahlen"; the standard translation of this term into English is " canal rays ". Wien found that the charge-to-mass ratio depended on the nature of the gas in the discharge tube. Thomson later improved on the work of Wien by reducing the pressure to create the mass spectrograph. Calutron mass spectrometers were used in the Manhattan Project for uranium enrichment. The word spectrograph had become part of the international scientific vocabulary by Once the instrument was properly adjusted, a photographic plate was inserted and exposed. The term mass spectroscope continued to be used even though the direct illumination of a phosphor screen was replaced by indirect measurements with an oscilloscope. Aston in and respectively. Sector mass spectrometers known as calutrons were developed by Ernest O. Lawrence and used for separating the isotopes of uranium during the Manhattan Project. In , half of the Nobel Prize in Physics was awarded to Hans Dehmelt and Wolfgang Paul for the development of the ion trap technique in the s and s. In , the Nobel Prize in Chemistry was awarded to John Bennett Fenn for the development of electrospray ionization ESI and Koichi Tanaka for the development of soft laser desorption SLD and their application to the ionization of biological macromolecules, especially proteins. This one is for the measurement of carbon dioxide isotope ratios IRMS as in the carbon urea breath test A mass spectrometer consists of three components: The ionizer converts a portion of the sample into ions. There is a wide variety of ionization techniques, depending on the phase solid, liquid, gas of the sample and the efficiency of various ionization mechanisms for the unknown species. An extraction system removes ions from the sample, which are then targeted through the mass analyzer and into the detector. The differences in masses of the fragments allows the mass analyzer to sort the ions by their mass-to-charge ratio. The detector measures the value of an indicator quantity and thus provides data for calculating the abundances of each ion present. Some detectors also give spatial information, e. Theoretical example[edit] The following example describes the operation of a spectrometer mass analyzer, which is of the sector type. Other analyzer types are treated below. Consider a sample of sodium chloride table salt. Sodium atoms and ions are monoisotopic , with a mass of about 23 u. Chloride atoms and ions come in two isotopes with masses of approximately 35 u at a natural abundance of about 75 percent and approximately 37 u at a natural abundance of about 25 percent. The analyzer part of the spectrometer contains electric and magnetic fields, which exert forces on ions traveling through these fields. The speed of a charged particle may be increased or decreased while passing through the electric field, and its direction may be altered by the magnetic field. The streams of sorted ions pass from the analyzer to the detector, which records the relative abundance of each ion type. This information is used to determine the chemical element composition of the original sample i. Surface ionization source at the Argonne National Laboratory linear accelerator The ion source is the part of the mass spectrometer that ionizes the material under analysis the analyte. The ions are then transported by magnetic or electric fields to the mass analyzer. Techniques for ionization have been key to determining what types of samples can be analyzed by mass spectrometry. Electron ionization and chemical ionization are used for gases and vapors. In chemical ionization sources, the analyte is ionized by chemical ion-molecule reactions during collisions in the source. Ionization occurs in the ion source. There are several ion sources available; each has advantages and disadvantages for particular applications. LC-MS , since at atmospheric pressure, the filaments used to generate electrons burn out rapidly. Thus EI is coupled predominantly with GC , i. GC-MS , where the entire system is under high vacuum. Hard ionization techniques are processes which impart high quantities of residual energy in the subject molecule invoking large degrees of fragmentation i. The most common example of hard ionization is electron ionization EI. Soft ionization refers to the processes which impart little residual energy onto the subject molecule and as such result in little fragmentation. Inductively coupled plasma[edit] Inductively coupled plasma ion source Inductively coupled plasma ICP sources are used primarily for cation analysis of a wide array of sample types.

In this source, a plasma that is electrically neutral overall, but that has had a substantial fraction of its atoms ionized by high temperature, is used to atomize introduced sample molecules and to further strip the outer electrons from those atoms. The plasma is usually generated from argon gas, since the first ionization energy of argon atoms is higher than the first of any other elements except He, O, F and Ne, but lower than the second ionization energy of all except the most electropositive metals. The heating is achieved by a radio-frequency current passed through a coil surrounding the plasma. Photoionization mass spectrometry[edit] Photoionization can be used in experiments which seek to use mass spectrometry as a means of resolving chemical kinetics mechanisms and isomeric product branching. Other ionization techniques[edit] Mass selection[edit] Mass analyzers separate the ions according to their mass-to-charge ratio. The following two laws govern the dynamics of charged particles in electric and magnetic fields in vacuum:

Chapter 5 : Interference's & Contaminants Encountered in Modern Mass Spectrometry

However,a mass spectrometer does not only serve as a machine for solving complicated analytical problems,it evolved meanwhile to a complete laboratory for the investigation of molecules,clusters,and other species under the environment-free conditions of the highly diluted gas phase.

Chapter 6 : Mass spectrometry: the most important analytical tool of modern times - The Hindu

In Modern Isotope Ratio Mass Spectrometry,the first comprehensive book written on the subject for twenty-five years, examples from all these areas, and many more,are given. All modern developments in this fascinating field are discussed with special attention paid to technical details and instrumentation.

Chapter 7 : Mass spectrometry - Wikipedia

Course Catalog Introduction to Modern Mass Spectrometry. This course covers mass spectrometry fundamentals as well as the latest developments in the field, with emphasis on biological and biochemical applications.

Chapter 8 : MS - Mass Spectrometry (MS) Beginner's Guide : Waters

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Chapter 9 : The Origins of Mass Spectrometry - The Analytical Scientist

However, one of modern mass spectrometry's great successes is the analysis of often low nanogram amounts of proteins separated and purified from complex mixtures with chromatographic or gel electrophoresis techniques.