Chapter 1 : Ion beam analysis - Wikipedia

Contents: Introduction to the physical basis of x-ray spectrometry and IBA methods -- XRS and IBA methods of surface analysis -- Applications of XRS and IBA methods as illustrated in studies on dental composites.

Fundamentals of Nuclear Physics and Engineering Fundamental: General properties of Nuclei: Constituents of nuclei, nuclear mass, charge and size, nuclear density, nuclear spin and angular momentum, nuclear binding energy, liquid drop model, statistics, mass formula Nuclear Structure: Nuclear Radius, The interaction between two nucleons, Nuclear models: Fission cross sections and threshold, the fission products, the mass and energy distribution of the fission products, neutron emission in fission, the theory of fission process, the energy distribution of the neutron emitted by fission, Fission in Stars Isotopes: Natural radioactivity and isotopes, isotopic masses and abundances: Transmutation by alpha particles, alpha-proton reactions, The neutron: Elements of Nuclear Engineering: The nuclear energy sources, Reactor Kinetics and Transfer function, The chain-reacting systems, Thermal nuclear reactor, The calculation of the multiplication factor for a homogenous thermal reactor, heterogeneous thermal reactor, the critical size of a thermal reactor, power and breeding, Fission and Fusion reaction, fission characteristics , Chain reaction, neutron transport and diffusion theory, diffusion and slowing down of neutrons, critical condition and critical concentration, mass and dimensions, reactor kinetics, one-speed one group and multi-group methods of neutron diffusion equations, analytical and numerical solutions of for neutron diffusion equations, fast and thermal spectrum calculations, inhomogeneous reactor design, effects of poisons and fuel depletion, Nuclear reactor dynamics and reactivity feedbacks, production and transmutation of radionuclide in nuclear reactors. Numerical Methods of Reactor Analysis: Computation methods to analyze nuclear reactor systems: Principles of Nuclear Reactor Design, Nuclear Reactor Core design, Principles and techniques of economic analysis to determine capital and operating costs, fuel management and optimization, thermal limits on reactor performance, thermal converters, fast breeders: Fusion reactions and cross sections, Fusion Reaction and Reactors, Engineering and design of fusion systems, introduction to controlled thermonuclear fusion as an energy economy, case study of fusion reactor design, engineering principles of support technology for fusion systems, Fuel Burn up, Tritium Breeding for Fusion Reactors, Tokomak reactors, magnetic mirror reactors, LASER driven reactors, economics of fusion reactors. Introduction to Reactor Physics, Riverhand. Nuclear Chemistry and Chemical Engineering Fundamental of Chemical Engineering and nuclear power industry, Build-up of heavy actinides, Burn-up and reactivity changes for mix and un-mixed fuel, Plutonium recycle, Nuclear fuel processing Solvent extraction, McCabe-Thistle diagrammatic solution of problems in separation process, Hafnium and Zirconium: Impotant Isotopes, Isotope effects and Separation of Isotopes, General cascade theory, Ideal, Close-separatio n and squared-off cascades, Separative duty, separation potential, Enrichment costs, Radiolysis of Water, Heavy water production, Uranium enrichment process: Countercurrent Separation Processes, Elsevier 3. Management of Nuclear Fuel Cycle and Reactor Thermal Hydrodynamics Foundation of nuclear fuel cycle with topics ranging from nuclear-fuel reprocessing to waste treatment and final disposal, the emphasis is on the relationship between nuclear-power utilization and its environment impacts. Mathematical models for individual process in a fuel cycle, waste solidification, repository performance and nuclear transmutation in a nuclear reactor, optimization of a fuel cycle. Thermodynamic analysis of nuclear power plants, non-flow, steady and unsteady flow, thermal analysis of fuel elements, thermal design and analysis of heat exchanger, steam generators and condensers. Nuclear Power System Engineering and Production of Energy Basics of nuclear power generation, Design, analysis and fabrication of nuclear powers systems, Energy conversion in nuclear power systems, thermal and structural analysis of reactor core and plant components, corrosion in nuclear power systems: Nuclear Analytical Techniques Geometry of Crystals Lattices, crystal systems, symmetry, primitive and non-primitive cells, lattice directions and planes, crystal structures, atom sizes and coordination, stereographic projection. Diffraction and Diffractrometer Introduction,

X-ray spectroscopy, diffraction directions, Laue methods, rotating crystal method, powder method, Diffractometer method, diffraction under non-ideal conditions, intensities of diffracted beams, scattering by an atom, scattering by a unit cell, structure factor calculation, multiplicity factor, Lorenz factor, absorption factor, Temperature factor, Intensities of powder pattern lines, Example of intensity calculations, counters counting losses, counting efficiency, energy resolution, proportional counter, scintillation counter, semiconductor counter, pulse height analyzer, energy-dispersi ve Diffractrometry , time analysis Diffractrometry. Qualitative and Quantitative Elemental Analysis: Neutron Powder Diffractometer, Neutron Scattering, Triple Axis Neutron Spectrometer, Characterizatio n of Functional materials, Study on the phase purity, lattice constants, phase fraction, phase transition, thermal vibration of atoms, long range and short range order, dislocation and defects in crystals, identification of light atoms in compounds, identification of atoms having close atomic numbers, identification of isotopes of the same element, micro structure materials, magnetic phase transition, orientation of the magnetic moments of atoms, magnetic disorder. Analysis of nuclear and non-nuclear materials, Detection of Defects, and corrosion in metals and alloys. Health Physics and Radiation Science Absorbed dose, radiation exposure, radiation-weigh ted dose units, Public health and radiation protection, philosophy of radiation protection, ICRP basic safety criteria, radiation dosimetry; Radiation hazards: Air sampling, continuous environmental monitoring; assessment of hazard-maximum credible accident, dose optimization. Paic, Ionizing radiation, protection and dosimetry, CRC press, National security and international law affairs: Principles and methods used in safety evaluation of complex engineered systems with principle emphasis on fission and fusion nuclear power plants, Safety philosophies regarding design, siting, operation and regulation, deterministic and probabilistic models and methods including seismic safety, fires and system safety. H Pigford and H W. Practical 2 Credit List of Practical Experiments 1. Measurement of Core Excess and Shutdown Margin. Measurement of the Reactivity Worth of a Control Rod.

The first of its kind, Introduction to Biophysical Methods for Protein and Nucleic Acid Research serves as a text for the experienced researcher and student requiring an introduction to the field. Each chapter presents a description of the physical basis of the method, the type of information that may be obtained with the method, how data.

Bring fact-checked results to the top of your browser search. Basic properties of atoms An isolated atom can be described in terms of certain discrete states called quantum states. Each quantum state has a definite energy associated with it, but several quantum states can have the same energy. These quantum states and their energy levels are calculated from the basic principles of quantum mechanics. For the simplest atom, hydrogen , which consists of a single proton and a single electron , the energy levels have been calculated and tested to an uncertainty of better than one part in , but for atoms with many electrons, the accuracy of the calculations may not be much better than a few percent of the energy of the levels. Atomic energy levels are typically measured by observing transitions between two levels. For example, an atom in its lowest possible energy state called the ground state can be excited to a higher state only if energy is added by an amount that is equal to the difference between the two levels. Thus, by measuring the energy of the radiation that has been absorbed by the atom, the difference in its energy levels can be determined. The energy levels are identical for atoms of the same type; allowed energies of a particular atom of silver are equal to those for any other atom of the same isotope of silver. Other isolated systems, including molecules , ions charged atoms or molecules , and atomic nuclei, have discrete allowed energies. The analysis of these simple systems is carried out with techniques that are analogous to those that were first applied to simple atomic spectra. More complex structures, such as clusters of atoms, and bulk condensed matter, such as solids and liquids , also have energy levels describable by quantum mechanics. The energy levels in these complex systems, however, are so closely spaced that they smear into a continuous band of energies. Transitions between these bands allow researchers to discern many important properties of a given material. The location and properties of the energy states are often referred to as the electronic structure of the material. If an atom in its ground state is given some amount of energy so that it is promoted to an excited state, the atom will release that extra energy spontaneously as it moves back into lower states, eventually returning to the ground state. For an isolated atom, the energy is emitted as electromagnetic radiation. Conversely, the relationship allows the energy states of an atom to be determined from measurements of its frequency or wavelength spectrum. The analysis of the discrete wavelengths emitted or absorbed by an atom or molecule was historically carried out using prism or grating spectrometers; because of the appearance of the separated light in these instruments, these discrete wavelengths are sometimes called spectral lines. Historical survey The basis for analytical spectroscopy is the discovery, made in by the German physicist Gustav R. Kirchhoff , that each pure substance has its own characteristic spectrum. These dark lines, sometimes called Fraunhofer lines , are also collectively referred to as an absorption spectrum. The spectra of materials that were heated in flames or placed in electric-gas discharges were studied by many scientists during the 18th and 19th centuries. These spectra were composed of numerous bright discrete lines, indicating that only certain wavelengths were present in the emitted light. They are called brightline, or emission, spectra. Although the possibility that each chemical element has a unique characteristic spectrum had been considered by numerous investigators, the early studies were hampered by the difficulty of obtaining relatively pure substances. Any sample could contain impurities that would result in the simultaneous production of many spectra. By using carefully purified substances, Kirchhoff demonstrated characteristic spectra and initiated the technique of spectroscopic analysis of the chemical composition of matter. Before the 20th century, there was no theory that could satisfactorily explain the origin of the spectra of the elements or the reason why different elements have different spectra. The quantitative understanding of the elemental spectra needed the development of a fundamentally new physical theory, and the spectra of the simplest atoms played the key role in the development of this theory. Many of the major developments in 20th-century physics were

motivated by an ever-increasing accuracy in the measurement of the spectra of the hydrogen atom; highlights include the discovery in by the Swiss scientist Johann J. Balmer that the frequency spectrum of hydrogen followed a simple numerical pattern, later revised by the Swedish physicist Johannes R. In the Danish physicist Niels Bohr presented the first theoretical model that could give quantized energy levels that were in quantitative agreement with measurements of the hydrogen spectrum. The Balmer series of hydrogen as seen by a low-resolution spectrometer. Schawlow, Stanford University, and Theodore W. Hansch, Max Planck Institute for Quantum Optics Despite the success of the Bohr theory in describing the hydrogen spectrum, the theory failed badly when applied to the next simplest atom, helium , which contains two electrons. It was also incapable of predicting the likelihood of transitions between energy levels. This theory, known as quantum mechanics , was extended by the Austrian-born Swiss physicist Wolfgang Pauli , the German physicist Max Born , and others. It has been remarkably successful in describing the spectra of complex atoms, ions, simple molecules, and solids. As the spectral lines of the hydrogen atom were measured with increased accuracy, greater demands were placed on the theoretical understanding of atomic spectra. The British physicist Paul A. Dirac combined quantum mechanics with the special theory of relativity in to describe particles moving close to the speed of light. His formulation of relativistic quantum mechanics provided an explanation for the so-called fine structure of the hydrogen spectrum see below Foundations of atomic spectra: Fine and hyperfine structure of spectra. In , the American physicists Willis Lamb and Robert Retherford discovered that the levels actually differ by roughly hertz see below X-ray and radio-frequency spectroscopy: In contrast, the transition frequency between the ground state and the first excited states was calculated as approximately 2. The theory, known as quantum electrodynamics QED , had its foundations in the discoveries of Dirac, Heisenberg, and Pauli. It is a complete description of the interaction of radiation with matter and has been used to calculate the energy levels of the hydrogen atom to an accuracy of better than 1 part in No other physical theory has the ability to predict a measurable quantity with such precision, and, as a result of the successes of quantum electrodynamics, the theory has become the paradigm of physical theories at the microscopic level.

Chapter 3 : Chemistry (CHEM) < North Dakota State University

Methods based on X-ray spectrometry The electronic transitions which give rise to X-ray emission spectra involve core electrons and are therefore relatively insensitive to the chemical and physical form of the determinant (Bertin,).

Chemical Concepts and Applications. Introduction to general and organic chemistry, with applications drawn from the health, environmental, and materials sciences. Chem Concepts and Applications Lab. General Chemistry I Laboratory. Matter, measurement, atoms, ions, molecules, reactions, chemical calculations, thermochemistry, bonding, molecular geometry, periodicity, and gases. Intermolecular forces, liquids, solids, kinetics, equilibria, acids and bases, solution chemistry, precipitation, thermodynamics, and electrochemistry. General Chemistry II Laboratory. Organic Chemical Concepts and Applications. Introduction to organic chemistry for pre-nursing and other students who need to meet the prerequisite for CHEM Principles of Chemistry I. Chemistry for students with good high school preparation in mathematics and science. Electronic structure, stoichiometry, molecular geometry, ionic and covalent bonding, energetics of chemical reactions, gases, transition metal chemistry. Principles of Chemistry II. Liquids and solids, equilibrium, kinetics, thermodynamics, acids and bases, oxidation-reduction chemistry, electrochemistry. Principles of Chemistry Laboratory I. Principles of Chemistry Laboratory II. Survey of Organic Chemistry. Structure and bonding, nomenclature; hydrocarbons: Organic Chemistry I Laboratory. First semester of a two-semester course in organic chemistry for students in sciences and pre-professional curricula. Organic Chemitry II Laboratory. Structure and reactivity, named reactions, carbon-carbon bond forming reactions, aromatic and heterocyclic chemistry, biomolecules and polymers, and multi-step synthesis. Majors Organic Chemistry Laboratory I. Organic functional group synthesis. Modern analytical tools for functional group analysis and structure determination. More advanced aspects of organic laboratory operations, synthesis, analysis, and structure determination using spectroscopic techniques. Mathematical and physical basis of chemical phenomena. Emphasis on quantum chemistry and spectroscopy. Emphasis on chemical thermodynamics. Includes discussion of chemistry topics, technical writing instruction and assignments; participation in senior seminar discussions. Electronic structure, ionic and covalent structure and bonding, point groups and symmetry, coordination chemistry, acid-base and redox chemistry. Geometric and space group crystallography. Structure and bonding in common minerals and industrially important solids. Analytical X-ray powder diffraction for qualitative and quantitative analysis of crystalline solids. Crystal structure analysis using powder methods. Introduction to X-ray fluorescence spectrometry. Methods of synthesis and characterization of inorganic and organometallic compounds. Analytical Chemistry I Laboratory. Chemical equilibrium and its analytical applications; introduction to chromatography and potentiometry. Theory and application of modern instrumental techniques, including spectroscopy and electrochemistry. Analytical Chemistry II Laboratory. Survey of the history of the chemical sciences from the stone-age through the early s. An interdisciplinary course designed for undergraduate students. Introduction to science and engineering of converting biorenewable resources into novel biobased materials and products. Introduction to principles and concepts critical to successful design of polymeric biomaterials, coatings, and biocomposites. Understanding environmental impacts through life cycle analysis LCA. Survey of Physical Chemistry. Conceptual approach to physical chemistry including thermodynamics, kinetics, and quantum mechanics. Application of fundamental concepts to the life sciences. Measurement of thermodynamic and spectroscopic properties of chemical substances, analysis of data. The object of the course is to enhance the knowledge of experimental and computational techniques in a sub area of physical chemistry. Introduction to Computational Quantum Chemistry. This is a mathematically non-rigorous introduction to procedures and capabilities of basic computational quantum chemistry with practical aspects on using common computational chemistry software. An interdisciplinary course designed for graduate students. Introduction to Chemical Research. This course will serve as an introduction to research in the molecular sciences, with the goal to prepare graduate students

for a successful graduate research experience and for a future research career in the molecular sciences. Chemical Applications of Group Theory. Symmetry, point groups, basic theory of mathematical groups, application of group theory to chemical bonding and spectroscopy. Advanced Survey of Inorganic Chemistry. This course is an advanced survey course in Inorganic Chemistry. It emphasizes structure, electronic and magnetic properties, bonding, and symmetry of inorganic compounds, including organometallic and coordination complexes, and their reactivities. Topics also include main-group chemistry, solid-state materials, Lewis acid-base chemistry, oxidation-reduction reactions, and an introduction to physical methods used to probe the properties and track reactions of inorganic compounds. Fundamental principles in photochemistry and photophysics, rules for electronic transitions, energy transfer, electron transfer, photochemical reactions of organic chromophores carbonyls, alkenes, enones, aromatics , singlet oxygen, photochemistry in organized and constrained media, organic solid state photochemistry, instrumental methods in photophysics, application of photochemistry. Synthesis, reactivity, and bonding in organometallic compounds. Physical Methods for Chemical and Biomolecular Research. Fundamentals and applications of physical methodologies, with emphasis on spectroscopic methods, used to probe molecular structure and the structural basis of reactivity. Covers optical, chirooptical, vibrational, paramagnetic resonance, and nuclear spectroscopic methods along with their applications to the study of molecular and biomolecular systems. Use of single crystal X-ray diffraction data to determine molecular and crystal structures. Theory of equilibrium chemistry in aqueous and nonaqueous systems; principles of chromatographic and other separation techniques. Theoretical basis and application of several modern chemical analysis techniques. The focus will be the application of electrochemistry, chromatography, electrophoresis, and mass spectrometry in the chemical and biochemical analysis. Design and operation of digital and analog circuits used in chemical instrumentation, computer interfacing. Theory and application of mass spectrometry in analysis, tandem mass spectrometry, ionization techniques. Physical Organic Chemistry I. Principles governing the reactivity of organic compounds and methods for determining reaction mechanisms. Physical Organic Chemistry II. Aromaticity, electrophilic substitution, Woodward-Hoffman rules. Radicals, carbenes, nitrenes, arynes, carbenium ions, survey of other reactive intermediates. Structure elucidation by spectrometric methods, including infrared, mass spectrometry, UV, and nuclear magnetic resonance. Interpretation of 2-D NMR spectra. Functional group synthesis, synthetic design, stereochemical control. Synthesis of heterocycles, aromaticity, organometallic chemistry, nucleosides, natural products. Total Synthesis of Natural Products. Retrosynthetic analysis, total synthesis, terpenes, alkaloids will be studied. Laboratory to accompany , with emphasis on NMR techniques. Fundamental principles of physical chemistry including quantum chemistry, spectroscopy, molecular thermodynamics, and kinetics. Macroscopic and microscopic models for the study of equilibrium properties of pure phases and solutions. Theory and practice of modern spectroscopic methods. Emphasis on visible and ultraviolet wavelength ranges. Experimental methods to determine reaction rates, empirical rate laws, transition state theory. Chemical physics of energy transfer and reactive collisions. Wave functions and their properties, quantum mechanical behavior of atoms and molecules. Ab initio and semi-empirical methods for the calculation of energetic and structural properties of molecules; computational methods.

Chapter 4 : High Definition X-Ray Fluorescence: Principles and Techniques

Note: Citations are based on reference standards. However, formatting rules can vary widely between applications and fields of interest or study. The specific requirements or preferences of your reviewing publisher, classroom teacher, institution or organization should be applied.

Interactive spectrum Widely used in both research and industry, infrared spectroscopy is a simple and reliable technique used for a variety of measurements and in quality control. It is especially useful in forensic science both in criminal and civil cases. Spectrometers are now small, and can be easily transported, even for use in field trials. With increasing progress in new technology, samples in solution can now be measured accurately water produces a broad absorbance across the range of interest, and thus renders the spectra unreadable without this new technology. Some instruments will also automatically tell you what a substance is by referencing it to a store of thousands of spectra held in storage. By measuring at a specific frequency over time, changes in the character or quantity of a particular bond can be measured. This is especially useful in measuring the degree of polymerisation in polymer manufacture or in identification of polymer degradation for example. The progress of formation of an epoxy resin being hardened by an amine cross linking agent can be monitored by observing the appearance of a hydroxy group in the spectrum of a polymerising sample or by the disappearance of an epoxy group. Modern research instruments can take infrared measurements across the whole range of interest as frequently as 32 times a second. This can be done whilst simultaneous measurements are made using other techniques. This makes the observations of chemical reactions and processes quicker and more accurate. Infrared spectroscopy has been highly successful for applications in both organic and inorganic chemistry. A second type of IR spectrometer is a dispersive spectrometer. The rotating mirror, M temporarily reflects the reference beam towards the machine optics whilst blocking the sample beam. Reference beam and sample beam are alternately blocked and reflected. The thermocouple converts the different wavelengths of IR reaching it to a signal which is represented as a spectrum. The difference between reference and sample signals shows which parts of the spectrum have been absorbed by the sample. In the FT spectrometer, an interferometer is used instead of a diffraction grating. The spectrum is obtained by a mathematical calculation a Fourier Transform. The FT spectrometer is more responsive, accurate and precise than a dispersive spectrometer. Advanced Chemistry â€" Energy Levels Two balls separated by a spring will oscillate harmonic if stretched and released. This model suggests that the spring will vibrate at any energy dependent on the initial separation of the balls but, this is not true for molecules. The energy is quantised, which means that only certain energy levels are allowed according to the formula: In addition, molecules can only absorb or emit energy equal to the spacing between two levels and, for a harmonic oscillation, this can only occur between adjacent levels. However, bonds in real molecules do not vibrate harmonically. When atoms approach each other closely, they exert a force of repulsion, and beyond a certain separation distance, a bond breaks. Quantisation produces unequal separations of energy levels which add complications to spectra. Finally, molecules will not absorb infrared radiation unless they possess a dipole, thus H_2 is transparent to infrared whilst HCl absorbs. Many molecules possess dipole moments due to non-uniform distributions of positive and negative charges on the various atoms e. These values can be obtained from measurement of the dielectric constant. When the symmetry of a molecule cancels out, there is no net dipole moment and the value is therefore 0. The highest dipole moments are in the range of 10 to Information about the molecular geometry of a molecule can be deduced from the dipole moment. For example the data indicates that carbon dioxide CO_2 is a linear molecule but ozone O_3 is not. Advanced Chemistry â€" More complicated molecules For non-linear molecules, for example pentane, there are a number of vibrations given by $3N$ â€" 6. N is the number of atoms in the molecule. Pentane , C_5H_{12}, 17 atoms has 45 different vibrations! Although there are a large number of vibrational modes here, the situation can be simplified by considering that each functional group can be considered independently. So a methyl group for example should have the same normal modes

of vibration no matter where it is located in a molecule. Carbon dioxide CO_2 is a linear molecule and produces just two peaks in the spectrum. This is because the symmetric stretch does not have a dipole and the two bending vibrations in plane and out of plane are degenerate i. The reason that only two peaks appear in the carbon dioxide spectrum is because the symmetrical stretching vibration does not have a change in dipole moment as it vibrates. The two bending vibrations are degenerate and vibrate at exactly the same frequency. Other simple organic molecules produce a large number of peaks which could be considered in terms of those vibrations which correspond to CH3, CH2, benzene ring and the main functional groups e. The following link shows the spin rotation of the aspirin molecule. The frequency for a C-H bond is approximately cm Advanced Chemistry â€" Types of Bonds Values of the force constant for a number of bonds are given in the table below.

Chapter 5 : Handbook Of Practical X Ray Fluorescence Analysis Book â€" PDF Download

Use of X-ray techniques in medical research Each chapter is written by one or more leading pioneers and experts in analytical chemistry. Contributions are based on a thorough review and analysis of the current literature as well as the authors' own firsthand experiences in the lab.

Applications[edit] Ion beam analysis has found use in a number of variable applications, ranging from biomedical uses to studying ancient artifacts. The popularity of this technique stems from the sensitive data that can be collected without significant distortion to the system on which it is studying. The unparalleled success found in using ion beam analysis has been virtually unchallenged over the past thirty years until very recently with new developing technologies. Even then, the use of ion beam analysis has not faded, and more applications are being found that take advantage of its superior detection capabilities. In an era where older technologies can become obsolete at an instant, ion beam analysis has remained a mainstay and only appears to be growing as researchers are finding greater use for the technique. Biomedical elemental analysis[edit] Gold nanoparticles have been recently used as a basis for a count of atomic species, especially with studying the content of cancer cells. Scientists have found an effective way to make accurate quantitative data available by using ion beam analysis in conjunction with elastic backscattering spectrometry EBS. The unique properties of ion beam analysis make great use in a new line of cancer therapy. Cultural heritage studies[edit] Ion beam analysis also has a very unique application in the use of studying archaeological artifacts, also known as archaeometry. What many have found useful in using this technique is its offering of excellent analytical performance and non-invasive character. More specifically, this technique offers unparalleled performance in terms of sensitivity and accuracy. Recently however, there have been competing sources for archaeometry purposes using X-ray based methods such as XRF. Nonetheless, the most preferred and accurate source is ion beam analysis, which is still unmatched in its analysis of light elements and chemical 3D imaging applications i. Current characterization is done based on heavy metals found in bullets, however, manufacturing changes are slowly making these analyses obsolete. The introduction of techniques such as ion beam analysis are believed to alleviate this issue. Software and simulation[edit] Dating back to the s the data collected via ion beam analysis has been analyzed through a multitude of computer simulation programs. Researchers who frequently use ion beam analysis in conjunction with their work require that this software be accurate and appropriate for describing the analytical process they are observing. As the purpose and implementation of ion beam analysis has changed over the years, so has the software and codes used to model it. Such changes are detailed through the five classes by which the updated software are categorized. This class of software solved specific problems in the data; niy did not provide the full potential to analyze a spectrum of a full general case. At the time, the computational models only tackled the analysis associated with the back-scattering techniques of ion beam analysis and performed calculation based on a slab analysis. A variety of other programs arose during this time, such as RBSFIT, though due to the lack of in-depth knowledge on ion beam analysis, it became increasingly hard to develop programs that accurate. Class-B[edit] A new wave of programs sought to solve this accuracy problem in this next class of software. This direct approach unfolds the produced spectrum with no assumptions made about the sample. Instead it calculates through separated spectrum signals and solves a set of linear equations for each layer. Problems still arise, though, and adjustments made to reduce noise in the measurements and room for uncertainty. Class-C[edit] In a trip back to square one, this third class of programs, created in the s, take a few principles from Class A in accounting for the general case, however, now through the use of indirect methods. RUMP and SENRAS, for example, use an assumed model of the sample and simulate a comparative theoretical spectra, which afforded such properties as fine structure retention and uncertainty calculations. In addition to the improvement in software analysis tools came the ability to analyze other techniques aside from back-scattering; i. Class-D[edit] Exiting the Class C era and into the early s, software and simulation programs for ion beam analysis were

tackling a variety of data collecting techniques and data analysis problems. Programs produced like SIMNRA now account for the more complex interactions with the beam and sample; also providing a known database of scattering data. Class-E[edit] This most recently developed class, having similar characteristics to the previous, makes use of primary principles in the Monte Carlo computational techniques. A key and popular feature that accompanies such techniques is the possibility for the computations to be incorporated in real time with the ion beam analysis experiment itself.

Chapter 6 : - NLM Catalog Result

The methods of X-ray crystallography are too complex to be described here; nevertheless, as automatic instrumentation and data handling techniques improve, it will undoubtedly prove to be the procedure of choice for structure determination.

Asymmetric placement of DCC monochromator crystal for beam spot magnification. Use of multiple DCC crystals to increase focused beam intensity. Schematic of rotationally wrap around DCC monochromators to increase focused beam intensity. The capture angle in the dispersive plane is typically 1â€"5 degrees and the rotational angle can be 5â€" degrees. The large solid angle of collection results in a monochromatic X-ray beam intensity produced with a low power 20â€"50 W X-ray source comparable to the intensity of a monochromatic beam obtainable from a high power 5â€"10 kW rotating anode source using conventional optics. As noted above, the focal spot size of the diffracted beam is mainly determined by the X-ray source size. The capabilities of commercially available DCC optics [34] are summarized in Table 3. Characteristics of current DCC optics. X-Beam Efficient use of DCC optics requires a close match between the optic and the electron bombardment X-ray source spot on the anode. As noted in Section 2 , for a well-made symmetrical toroidal optic, the source spot size is imaged at the optic focal point. For asymmetrical optics and for optic figures different from circular toroidal optics, a more complex relationship between the source spot size and the image focal spot size exists. For example, the focal spot for an inverse logarithmic spiral optic of the type shown in Figure 7 is much larger than the source spot size. For some applications this is acceptable, especially if the detector used has an input area larger than the spot size. It should be noted that it is not possible to reverse this optic in order to achieve a small spot size from a large source since X-rays from each part of the source are incident on each part of the optic. Virtually in every application, precise alignment of the optic with the source position is critical. This can often be a problem since the source spot position on the anode can vary as the source warms up or if the source power is changed, causing the alignment to change and the optic output intensity to vary. To alleviate this problem, proprietary X-beams have been developed at XOS in which a thermal management system is used to keep the source spot constant during warm up of the source which in some cases can take as long as two hours or the source power is changed. In the X-beam assembly, the optic is prealigned and the desired beam intensity can be obtained within less than two or three minutes and held constant usually within 0. Furthermore, the desired intensity can be reproduced through multiple on-off cycles of the X-ray system. In addition, X-Beams are internally shielded against radiation leakage and can contain an internal shutter and filter wheel assembly. Also, X-Beams with coupled DCC optics are air cooled, compact, and can be operated in any arbitrary orientation. A typical DCC X-Beam, about eight inches high and weighing less than five kilograms, is shown in the inset in Figure 9. This compact, low-power, safe, rugged, and reliable X-ray source-optic assembly is at the heart of most HD XRF analyzers discussed in the accompanying paper [31]. Fundamental Parameters Analysis The ability to measure the intensity of X-ray fluorescence from individual elemental constituents in complex materials even when the amount present is low provides the possibility for rapid, nondestructive elemental analysis. As shown in Figure 1 , such measurements are greatly facilitated by the use of a monochromatic excitation beam. This has been recognized for decades. For very thin samples such as for air particulates collected on thin filters, quantitative analysis is straightforward. Such first principle calculations for thin samples require measurement of the integrated peak intensity for each element and application of experimentally determined detector response functions and experimental [35] or calculated [36] fluorescent X-ray yields for pure samples of the elements of interest for a monochromatic excitation X-ray beam of the appropriate energy. The excitation probability is highest for elements with fluorescent X-rays just below the energy of the exciting photons. For accurate measurement, it is still necessary in such measurements to make corrections for absorption and scattering from the measured elements and from the filter collector. For thicker samples, matrix scattering and absorption effects become

much more important and suitable corrections and adjustment are crucial for quantitative application of X-ray fluorescence. Experimental X-ray excitation curve measured for a Zr secondary source by the use of thin metal samples evaporated on thin Mylar substrate films from [35]. Since the seminal work of Compton [38], methods have been explored to make matrix corrections for X-ray fluorescence analysis. These have traditionally involved use of standards of known composition [39 , 40] to calibrate the measurement system which must always take into account the detection method, geometry, and sample form. For conventional X-ray fluorescence, the analysis is complicated by the presence of a large Bremsstrahlung continuum which also reduces measurement sensitivity and requires background evaluation methods [41 , 42]. The clean, background-free X-ray spectrum also permits analysis of the ratio of the Rayleigh coherent and Compton scattering incoherent peaks for evaluation of X-ray absorption and scattering due to elements in the sample matrix. This is particularly important in evaluating the matrix effects from light elements such as H, C, N, and O that are not measured in the XRF spectrum. A comprehensive review of studies based on the use of the Compton scattering, especially for monochromatic secondary and radioactive sources, is given by Nielson [43]. A detailed analyses for matrix absorption and scattering effects for fundamental parameter FP analysis of a variety of materials from low Z substrates such as petroleum to plant, mineral, and metal substrates using single Zr [44] and double Zr and Ti secondary X-ray sources [45] is described by Nielsen using an iterative analysis procedure [35]. An HD XRF analysis software package built upon and extending the previous work is currently under development at XOS based on the fundamental parameter approach [46]. This fundamental parameter FP approach has already achieved notable success in analysis of thin, filter or impact membrane collected air particulate samples. As discussed in the accompanying paper, the use of HD XRF is particularly valuable for measurements of small particle fractions of importance for health studies and for the small sampling volumes and small sample sizes needed for portable personal environmental monitors. Measurement of ultratrace element concentrations in calibration samples prepared and characterized at the Trace Elements Laboratory at Wadsworth Center of the New York State Health Laboratory for evaluation of body fluids urine, blood, and plasma has shown excellent agreement with inductively coupled plasma-mass spectroscopy ICP-MS characterized samples for lead and arsenic at concentrations from 10 ppb to less than 50 ppb. Computer-based simulations are very useful to understand the X-ray scattering and absorption processes and the role of detector response functions and measurement geometries that lead to monochromatic EDXRF spectra for a variety of analyte elements over a wide range of concentrations in different sample matrices and thicknesses. This has been abundantly demonstrated in an extensive systematic program based on a Monte Carloâ€"Library Least-Squares method developed by Gardener et al. A detailed summary of this method is given by Li et al. An example of such a simulation for a polyethylene standard sample containing controlled amounts of Cr, Hg, Pb, and Br is shown in Figure This simulation is being refined to more completely account for secondary scattering effects. Analyses of thick plastic standards are shown in Table 4 with concentrations of observed heavy element constituents obtained from fitting of simulated peak intensities as shown in Figure Even without further refinement, agreement with the reference values is very close and provides a basis for reverse FP analyses for thin or thick water or plastic-matrix homogeneous samples. The analysis is currently being refined for other plastic, organic, or metallic homogeneous matrices. Reference and measured values for three polyethylene standards. A background subtraction was made for the spectrum below The physical constants used in the FP analysis are the incident and exit angle, the energy of the incident monochromatic X-ray beam, tabulated mass attenuation coefficients [55], fluorescence yields [56], absorption jump ratios [57], intensity ratios of lines within a given series e. The effects of particle size in inhomogeneous matrices and samples with layers of differing materials and constituents are under examination. A special but important class of layered inhomogeneous samples is paint on a thick homogeneous substrate. Both experimental and analytical studies are underway for FP analysis of such cases. Preliminary results show promise for such applications and are discussed in the accompanying paper on HD XRF applications [31]. Conclusions A new HD XRF system based on the use of proprietary DCC X-ray

optics coupled with low-power X-ray tube sources in a proprietary, compact, portable, safe, stable, X-beam assembly for monochromatic, microfocus, energy dispersive, X-ray fluorescence enables a broad variety of in situ, online, clinical, or remote applications in science, medicine, and industry. The principles and techniques as well as the basis for automated fundamental parameter FP standardless analysis that is enabled by this new analytical tool are discussed in this report. Selected applications are reviewed in an accompanying paper [31]. Development of specialized HD XRF analyzers based on this approach is discussed in the companion paper [31]. The content is solely the responsibility of the authors and does not necessarily represent the official views of the Department of Energy, the National Institutes of Health, the National Science Foundation, or the Environmental Protection Agency. The authors would also like to acknowledge discussions and active participation with colleagues at X-Ray Optical Systems, Inc. Van Grieken and A. View at Google Scholar K. View at Google Scholar W. View at Google Scholar J. View at Google Scholar B. View at Google Scholar S. View at Google Scholar P. Siddons, Handbook of Optics, Vol. View at Google Scholar D. View at Google Scholar Z. View at Google Scholar A. View at Google Scholar R.

Chapter 7 : Introduction to Spectroscopy - SpectraSchool

Introduction to Biophysical Chemistry Ch 24a discusses the interaction of light with matter (absorption, emission, scattering), methods of identification of macromolecules (absorption spectroscopy, mass spectrometry), methods of.