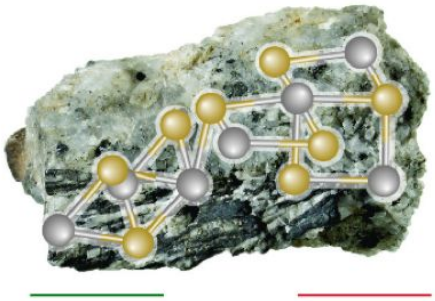

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SMCr

SMCr. VI Reunión Nacional de Difractometría
I Reunión Internacional de Radiación Sincrotrón
Reunión de Usuarios de Luz Sincrotrón
6-8 de noviembre de 2019. UAEH, Pachuca de Soto, Hidalgo, México.

Some Examples of Diffraction Studies on Complex Inorganic Materials

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Abstract. In this talk a selection of studies on complex inorganic materials - of synthetic as well as natural origin - will be presented. In the first part, examples of traditional in house X-ray diffraction studies will be discussed, however on materials with less common chemical composition, in particular involving actinoid elements. The second part describes cases for which specific properties of synchrotron radiation had to be exploited, in particular wavelength tunability. The last part deals with very complex natural minerals which occur only as nanoscopic samples and thus require the newly developed method of electron diffraction tomography (EDT). These materials are ordered only on the nanometer scale and their structures are therefore largely inaccessible for traditional diffraction methods.

Keywords: Laboratory X-ray diffraction, synchrotron radiation uses, electron diffraction tomography.

Acknowledgements. Financial support by the Mexican Society of Crystallography, A.C. (SMCr, A.C.), the National Council for Science and Technology (CONACYT, Mexico) and the Deutsche Forschungsgemeinschaft (DFG, contract number DE412/49-1) is gratefully acknowledged. I am also indepted to all my colleagues and co-workers for their collaboration over so many years.

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VI REUNIÓN NACIONAL DE DIFRACTOMETRÍA

Intra- and intermolecular interactions in heterocyclic tin compounds

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Abstract. It is well known that heavier group 14 elements have the ability to expand their coordination numbers above four, accommodating formally more than eight electrons in their valence shell to form so-called hypervalent compounds.[1] To promote this bonding situation, ligands capable of yielding compounds containing chelate rings, by means of an acceptor-donor intramolecular bond, have been used in order to increase the coordination number of an acceptor atom **A**.[2] The diverse nature of the exocyclic ligands linked to **A** affects the strength of this **A---D** interaction, and also promotes several intermolecular interactions.
Here, some structural results of compounds having heavier group 14 elements will be presented. The studies were carried out by X-ray single-crystal diffraction experiments, in order to analyze the different intra- and intermolecular interactions; the type and nature of these interactions are presented and discussed.

Keywords: Tin compounds, Hypervalent compounds, X-ray studies

Acknowledgements. The financial support of CONACYT and UAEH is gratefully acknowledged; I also want to thank the SMCr for the invitation.

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VI REUNIÓN NACIONAL DE DIFRACTOMETRÍA

Neutron protein crystallography: A complementary tool for locating hydrogens in proteins

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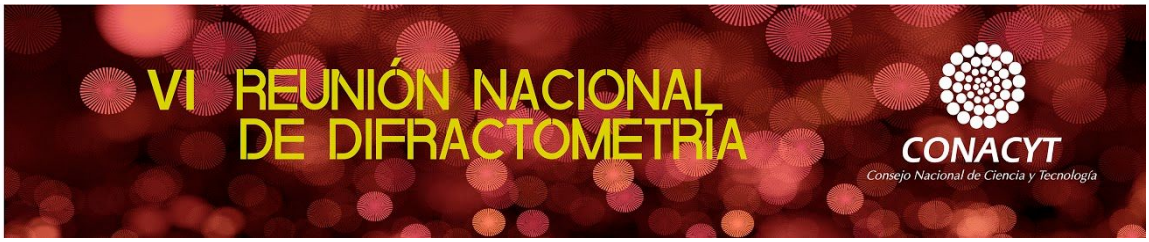
Abstract: From the early neutron diffraction experiments with protein crystals in the 1970s, neutron protein crystallography (NPC) has matured into an impactful experimental approach for directly observing hydrogen (or deuterium) atoms in protein structures. NPC provides the unrivaled capability to refine independently the atomic coordinates of hydrogens involved in protonation/deprotonation, oxidation/reduction and proton/hydrogen transfer enzymatic mechanisms based on observed reflections at medium crystallographic resolutions (≤ 2.5 Å). In this presentation, I will review the capabilities and practical considerations of NPC and also present recent scientific examples highlighting the complementarity of NPC with other experimental techniques routinely employed to locate hydrogens in proteins.

Keywords: neutron diffraction, macromolecular crystallography, protein structure.

Acknowledgements. This work has received support from the US National Science Foundation (1069091), the US Department of Energy, Office of Basic Energy Sciences and the National Institute of Standards and Technology, US Department of Commerce. The author acknowledges support to attend this meeting from the Mexican Society of Crystallography, A.C. (SMCr, A.C.), and the National Council for Science and Technology (CONACYT, Mexico).



Structure determination of Pharmaceutical Materials using X-ray Powder Diffraction Data

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Abstract.

For several decades Single Crystal X-Ray Diffraction has consistently provided the most reliable information on the 3D disposition of the atoms and molecules of materials of very diverse nature, from minerals to proteins. The possibility of having a suitable single crystal is certainly a limiting factor for the use of such a powerful technique. In certain cases, the structural characterization of a given material is needed as powdered sample as it is used in a technological application. To overcome the severe loss of information arising from the serious Bragg peak overlap recorded in Powder Diffraction patterns, an increasing array of powerful methodologies, implemented in many public domain programs, have facilitated the process of determining reliably the crystal structure of many important materials. Nowadays it is possible to obtain structural information from powder diffraction data which until recently was believed to be possible to obtain only from single crystal diffraction techniques.

In this contribution, several examples of pharmaceutical compounds studied by undergraduate and graduate students of our research group will be presented. Among the most interesting examples are phases of Thiocolchicoside (a muscle-relaxant drug used in the treatment of orthopedic, traumatic and rheumatologic disorders), Trichlormethiazide (a diuretic drug used in the treatment of hypertension), Sulbutiamine (a derivative of vitamin B1 used in the treatment of asthenia), Flunixin (a nonsteroidal anti-inflammatory, analgesic and antipyretic veterinary drug), Oxamic acid (an inhibitor of Lactate dehydrogenase A), among others.

Keywords: Crystal Structure determination, Powder Diffraction Data, Pharmaceuticals.

Acknowledgements: One of the authors (JMD) is very thankful to The Mexican Society of Crystallography (SMCr, A. C.) as well as the National Coincil for Science and Technology (CONACYT, Mexico) for the support to attend this meeting.

New Trends in Synchrotron Radiation at the NSLS-II

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Abstract

The highly Automated (AMX) and Frontier (FMX) macromolecular crystallography beamlines at the NSLS-II (BNL, Upton, NY, US) are in general user operation mode since a little less than three years now. These 2 beamlines represent the state of the art of what's currently available to the worldwide community in terms of beam brightness. The beamlines as well as scientific computing and sample automation will be presented. These beamlines can be operated in various modes including automated mode. Scientific highlights enabled by these 2 beamlines will be presented.

Keywords: Macromolecular Crystallography, Micro-focus, micro crystals, automation, pixel array detector, rastering, vector, high throughput, remote data collection, high capacity, multiple-crystals, serial crystallography.

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VI REUNIÓN NACIONAL DE DIFRACTOMETRÍA

On the applications of synchrotron light

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Abstract. Dedicated sources of synchrotron light have been available since the early seventies. Since many technological developments has enabled forefront discoveries. Major applications continue to in condensed matter physics, material sciences, chemistry, biology and medicine. Most of the research performed at synchrotron sources probe the structure of matter from sub-nanometer to the millimeter level. In this talk I will discuss some of the applications of synchrotron radiation and its true inter-disciplinary character.

Keywords: Diffraction, X-rays, Complementarity Methods.

Acknowledgements. I am most grateful to the Mexican Society of Crystallography, A.C. (SMCr, A.C.),The Institute of Materials Research (IIM) at UNAM, and the National Council for Science and Technology (CONACYT, Mexico) for their support. The Center for Biomolecular Structure is supported by a National Institute of General Medical Sciences (NIGMS) P30 grant, and by the DOE Office of Biological and Environmental Research (BER). The National Synchrotron Light Source II, a U.S. Department of Energy, DOE, User Facility is operated under Contract No. DE-SC0012704.

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The Use of Synchrotron Radiation in Environmental Sciences

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Abstract. In Environmental Sciences, the speciation of potentially toxic elements plays an important role in the study of the risk assessment that potentially toxic elements have in the environment. It is important to determine the species found in the environment of Potentially Toxic Elements (PTE), because the chemical species determines their distribution in the environment and its toxicity. Speciation, according to the IUPAC (International Union of Pure and Applied Chemistry) is the distribution of an element among certain well-defined species in a system. Identifying and quantifying these species represents a challenge in Analytical Chemistry. Therefore, different methodologies have been developed over the years for speciation analysis. X-ray Absorption Spectroscopy (XAS) is a method used for this purpose due to different advantages it presents to perform the speciation of potentially toxic elements in the environment. XAS is a highly sensitive technique, with detection limits in the tens of micrograms/g makes it especially useful in environmental sciences. In addition, it can be carried out in solids (crystalline and amorphous), as well as liquids without the use of sample extraction or preparation procedures.

XAS is widely used in chemical speciation, not only in environmental sciences, but also to analyze samples from health and material sciences. For XAS study, the distinction between XANES and EXAFS should be made. The XANES (X-ray Absorption Near Edge Spectroscopy) allows to know the oxidation state of the elements and their hybridization, while the EXAFS (Extended X-ray Absorption Fine Structure) provides structural information of the element under study, such as interatomic distance and coordination number which are very important to detect small changes in the chemical environment of the elements.

Synchrotron radiation is necessary for XAS studies and therefore this work shows the advantage of using synchrotron radiation in the analysis of environmental materials. In addition, different cases are shown where the study of different potentially toxic elements such as Pb, As, Se, Hg, Cd, Cu, Zn among others that are found in contaminated sites around the world and in Mexico is carried out. Finally, the advantages of using XAS for the analysis of PTE in different environmental matrices such as soil, mine tailings, particulate matter, nanomaterials, plants and some other biological tissues are shown.

Keywords: speciation, metal, toxicity, XAS, XANES, EXAFS

Acknowledgements. Thanks to the Mexican Society of Crystallography, A.C. (SMCr, A.C.), and the National Council for Science and Technology (CONACYT, Mexico).

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VI REUNIÓN NACIONAL DE DIFRACTOMETRÍA

Structure of Metal Derivatives of Active Pharmaceutical Ingredients

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Abstract.

Many Active Pharmaceutical Ingredients (APIs) are formulated as metal salts or complexes due to enhanced solubility and bioavailability of the metal derivative. Metal complexation may also help improve stability during manufacturing, storage, and transport. Additionally, it has been well-established that a metal derivative of an API can either potentiate or inhibit the therapeutic effect of the API and reduce or increase undesirable side effects. For these reasons, research on the potential use of salts or complexes continues to be a very active area for the development of new drug formulations.

For several years, one of our research interests has centered around the crystal chemistry of metal salts and complexes of APIs which contain carboxylate groups and other substituents which can easily coordinate to metal atoms. The structures of several metal derivatives of fluconazole, gluconic acid, γ-aminobutyric acid, valproic acid, and mefenamic acid prepared in our laboratory will be discussed.

Acknowledgements. We thank Licds. J. Trejo and Y. Escalante (ULA-Venezuela). We are also grateful to Prof. J.A. Henao and Dr. R.A. Toro (UIS-Colombia) and Prof. H. Camargo (UST-Colombia). One of the authors (GDD) is very thankful to Mexican Society of Crystallography (SMCr, A.C.) and the National Council for Science and Technology (CONACYT, Mexico) for the support to attend this meeting.

Keywords: Crystal Structure determination, Metal complexes, Pharmaceuticals.

VI REUNIÓN NACIONAL DE DIFRACTOMETRÍA

Advances in the strategic planning of the Mexican Light Source

Brenda Valderrama[1], **Víctor del Río**[2], **Juan García-Godínez**[3], **Balfre Sánchez-Roldán**[1,3], **Mireya Gally-Jordá**[1,3], **and Lamán Carranza**[3]

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Abstract. The purpose of this talk is to present the advances associated to the strategic planning of a large scientific facility in Mexico such as the Mexican Light Source. This planning is divided into three operative stages: design, construction and operation and involves site validations, conceptual design of the accelerator, detailed engineering, architectural design and construction supervision, all performed by multinational teams. At the same time, it is necessary to generate programs to support current and potential users, outreaching activities aimed to undergraduate and graduate students as well as regular feeds for the public opinion and politicians in Hidalgo. We will also present how we have dealt with the intricate administrative procedures related to the creation and operation of an office without precedent in the local government. Furthermore, it is absolutely important to keep the scientific community informed about the aims and opportunities of the project. All this would be impossible without the close collaboration and support from an interdisciplinary team leaded by the Government of Hidalgo under the structure of Scientific Advisory Committees. Currently, the project is on route and is expected to be completed in time.

Keywords: Mexican Light Source, Sincrotrón Mexicano en Hidalgo.

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The Mexican Synchrotron Light Source: Newest generation and its characteristics

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Abstract

An Advanced Synchrotron Light Source (ASLS) is a multipurpose and ubiquitous tool of present-day science. Indeed, there are about fifty such facilities of this kind around the world. The most advanced economies in the planet have several SLS and an increasing number of developing countries that wish to attain a superior level of scientific, technical, cultural and humane have one or are in the process of building its own SLS. Among the first 15 largest economies Mexico is the only one lacking an ASLS. In November of 2018, one year ago, the Government of the State of Hidalgo Mexico took the initiative of promoting a Mexican Synchrotron Light Source (MSLS). Hidalgo´s government promised to take three important steps toward this goal: to support the start of the MSLS with 25 million USD as a seed budget, a suitable piece of land of at least 40 hectares to build the project and most decisively to support and lobby to secure the political and financial support for the project. In this talk, I will present some recent applications, advances in the conceptual design and international support for this project.

Keywords: synchrotron, ASLS, MSLS,

Acknowledgements. The author (MM) acknowledges the Mexican Society of Crystallography, A.C. (SMCr, A.C.) as well as CONACYT for the support to attend this meeting.

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Exploring Allergies through Structural Biochemistry

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Abstract

Hypersensitivity reactions mediated by immunoglobulins E (IgE) are considered an important public health problem in the industrialized world and an increased prevalence has been reported in developing countries. Asthma and allergic rhinitis are major diseases in Mexico. Natural rubber latex (NRL) from *Hevea brasiliensis* contains several proteins involved in this type of allergies. These proteins are mainly implicated in plant defense mechanisms and are also involved in cross-reactivity against fruits, pollens, and insect venoms. Scarce structural information about this type of protein is available, and the cascade of events leading to symptoms is also poorly understood. Among NRL allergens, there are β-1,3-glucanases (Hev b 2), lectins (Hev b 6.02), class I chitinases (Hev b 11), and profilin (Hev b 8). We have solved the crystal structure several NRL allergenic proteins. Besides, we have produced several murine monoclonal antibodies IgG and a novel IgE (mAb 2F5), specific for profilin that will help us to identify epitopes [1]. Our results provide evidence that profilin dimerization considerably increases the IgE-mediated degranulation in rat basophilic leukemia cells and demonstrate the presence of allergen-specific patches consisting of a relatively high proportion of surface-exposed aromatic residues. Recently, we have obtained crystals of the complex Fab-IgE 2F5-profilin that show the epitopes involved in recognition of this antigen, which contribute to the elucidation of the etiology of this problem, and the development of strategies for diagnosis and treatment.

Keywords: Allergy, hypersensitivity, immunoglobulins E, latex, *Hevea brasiliensis*, chitinases, profilin.

Acknowledgements. One of the authors (A.R-R) acknowledges supported from the Mexican Society of Crystallography, as well as the National Council for Science and Technology (CONACYT, Mexico). This work was supported by DGAPA-UNAM (IN208418) and CONACYT 299048

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X-ray crystallography and electronic fluxes, implications on catalysis and environmental adaptations in proteins.

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Abstract. The field in which the academic development of our Research Group is focused is Structural Biology. In this area, the description and understanding of the operation at the atomic level of different proteins and enzymes requires a multidisciplinary approach in which the 3D structure is important but not sufficient. In the 80s of the last century, the idea arose that the 3D description of a protein was sufficient to describe and understand the catalytic mechanism and its implications. Although there were several cases with functional results, there are many examples in which the mere 3D description was insufficient to fully describe the enzymatic process, and even more so when this 3D description is based solely on X-ray diffraction data of crystals, that is, the main reason for these failures is due to the use of a single technique during the descriptive process. In our Group, we use an integrative approach of various techniques to unravel the enzymatic behavior and other proteins at the atomic level, and in some cases even at the subatomic level. The use of techniques of Molecular Biology, Microbiology, Biochemistry, Crystallogenesis, X-ray Diffraction, NMR, microPIXE, EPR, UV-Visible Spectroscopy, RAMAN, CD, SAXS, among others, is common within the group, generating detailed results and even subatomic levels, in various protein systems, especially in those where the presence of metal centers. In the first stage, this type of approach was used in enzymes with Fe and/or Cu (laccases and peroxidases), however, this approach has and will continue to be expanded following the development of the group's projects, both in metalloenzymes and in another type of enzymes. The development of the group has led to an expansion of the research lines and as a result of this we are currently working on the function and characteristics of protease inhibitors; the structural relationships between poisons and antibodies; the structural characteristics that confer resistance to high doses of ionizing radiation to certain microorganisms; the structural characteristics of enzymes that confer resistance against antibiotics; several studies in order to reduce the intrinsic damage of exposure to X-rays; the structural relationships in proteins involved in biomineralization processes; the structural determinants that confer the biofluorescence characteristic to several proteins similar to the green fluorescent protein; the mechanisms of transport of metals in microorganisms and the structural study of proteins that allow several species of shrimp to survive in highly contaminated habitats. All these approaches have a common axis, the study and consolidation of

Structural Biochemistry as a guiding area of modern approaches to problems from basic to apply in Biochemical Sciences. The development of this area of Structural Biochemistry has allowed us to achieve local and international recognition, with a large number of postgraduate students with more than 130 crystallographic structures determined and deposited in the PDB.

Keywords: Protein Crystallography, Synchrotron Radiation, Structural.

Acknowledgements. Author acknowledge the Mexican Society of Crystallography, A.C. (SMCr, A.C.) for the forum and invitation and IBt Institutional budget, the National Council for Science and Technology (CONACYT, Mexico) and his economic incentive from SNI for financing his research.

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Cristalografía de proteínas y el diseño racional de anticuerpos

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Abstract. Antibodies recognize and interact with proteins and other biomolecules with great affinity and specificity. However, its post-translational modifications and the presence of intrinsic disulfide bonds present difficulties for its industrial use. The immunoglobulin domain is one of the most ubiquitous folds in nature and is found in many proteins in addition to antibodies. In this work we use a cysteine protease inhibitor as a platform or scaffold to design novel proteins that mimic protein-protein interactions. The above because said protein does not contain any cysteine in its amino acid sequence. As proof of concept we use a variant of this inhibitor to mimic the interaction between the transcription factor p53 and its main regulator that is the MDM2 ubiquitin ligase, which is used as a biomarker in several types of cancer. Through protein engineering, we were able to modify the surface of our scaffolding and we managed to make it interact with the MDM2 biomarker. The designed proteins (chimeras) form a stable complex with an affinity similar to the canonical interaction between the p53 and MDM2 proteins. The molecular structure by X-ray diffraction of one of the chimeras in complex with MDM2 reveals that the modified region of the scaffold that interacts with MDM2 mimics the interface between a monoclonal antibody and MDM2. That is, we are able to produce a novel protein that has the recognition function similar to that of antibodies. The potential of our work in the area of bionanotechnology is relevant in various fields such as therapeutic, the detection of conditions such as cancer (biosensors), and in the separation of biomolecules with industrial possibilities. We continue to develop this technology to design biosensors against other relevant viruses, fungi and bacteria proteins

Keywords: Antibodies, MDM2 ubiquitin ligase, protein p53, X-ray diffraction.

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New approaches in electron diffraction to solve the structure of nanostructured materials

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Abstract. In the field of nanotechnology defining the atomic structure of a material is of paramount importance in order to understand its properties. In general, the structure of regular solids can be determined via conventional methods like X-ray, neutron, or electron diffraction. In this case, the order in the structure displays long-range characteristics with repeating units that do not vary considerably over the atomic and molecular scale. Electron diffraction has been used for several decades to identify crystalline structures, identification of group symmetries, and structural defects. However, in electron diffraction, the multiple scattering interactions result in spurious reflections and non-proportional intensities of the electron diffraction patterns, which cannot be supported by the kinematical framework. In order to address this issue, precession electron diffraction (PED) gives an alternative to overcome this problem by changing the beam orientation, so that at any moment few beams are excited simultaneously, resulting in a sizable reduction of dynamical effects. In the present talk, the advantages of PED will be covered to study the nanostructured and grain boundaries. A correlation between PED patterns and images registered by off-axis electron holography will be shown. The second part of the talk will address the structural analysis of materials using the pair distribution function (PDF) method, which has been commonly used using x-ray diffraction. Electron diffraction has the advantage to register the patterns at individual nanocrystals. Most of the crystalline phases can be inferred by conventional selected area electron diffraction. However, due to highly dynamical effects caused by the great interaction of electron with matter, it is usually not possible to obtain kinematical diffraction patterns. For this reason, X-rays are still widely used especially for solving crystal structures. In the present work we collected electron diffraction patterns with an axial CMOS (16 bit) camera under precession electron conditions. The patterns have registered and post-processed with ePDF software and SUePDF. Quantification with theoretical models have been performed with Diffpy for fitting, using python libraries.[1,2] Samples tested have been fcc gold decahedra, ligand-protected gold nanoparticles and the subtraction of the amorphous carbon contribution. PED-PDF measurements open a new door to study the structure of of non-translational symmetry nanostructured materials using a transmission electron microscope rather than the synchrotron X-ray sources.

Keywords: precession electron diffraction, nanobeam diffraction, pair distribution function

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