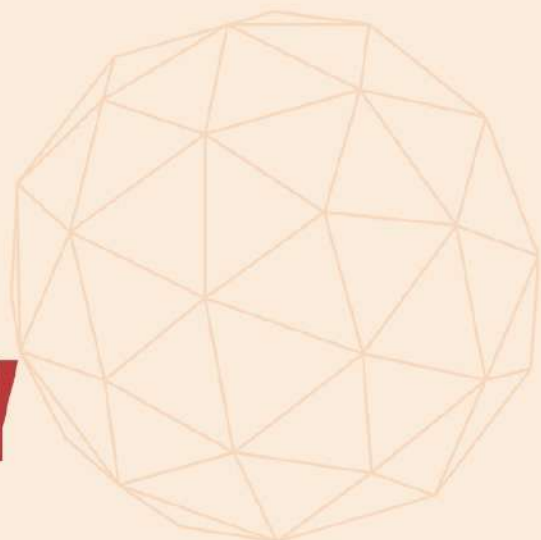


International School on  
**FUNDAMENTAL  
CRYSTALLOGRAPHY**



**7<sup>th</sup>** MaThCryst School in Latin America  
**LIMA, PERU, AUGUST 12 - 16, 2024**

**ABSTRACT BOOK**

[www.even3.com.pe/e/ISFC2024-7MathCrystS](http://www.even3.com.pe/e/ISFC2024-7MathCrystS)





**7<sup>th</sup> MathCryst**  
**In Latin America**



# **INTERNATIONAL SCHOOL ON FUNDAMENTAL CRYSTALLOGRAPHY**

**INTERNATIONAL SCHOOL ON FUNDAMENTAL CRYSTALLOGRAPHY**

SEVENTH MATHCRYST SCHOOL IN LATIN AMERICA

Lima, August 12<sup>th</sup> to 16<sup>th</sup>, 2024

ABSTRACT BOOK

[www.even3.com.pe/e/ISFC2024-7MathCrystS](http://www.even3.com.pe/e/ISFC2024-7MathCrystS)

# CONTENT

ABOUT THE SCHOOL	4
ORGANIZING COMMITTEES	5
REVIEW SYSTEM	6
GENDER EQUITY AND DIVERSITY POLICY	6
DATA OF THIS EVENT	8
LECTURERS	9
TUTORS	10
LANGUAGE	10
PROGRAM FIRST DAY 12TH AUGUST 2024	11
PROGRAM SECOND DAY 13TH AUGUST 2024	13
PROGRAM THIRD DAY 14TH AUGUST 2024	14
PROGRAM FOURTH DAY 15TH AUGUST 2024	16
PROGRAM FIFTH DAY 16TH AUGUST 2024	18
A Parallelizable X-Ray Diffraction Pattern Simulation for Fast Rietveld Refinement	20
Atomic structure of the $i\text{-Al}_{64}\text{Cu}_{23}\text{Fe}_{13}$ aperiodic crystal and its application as a mechanical reinforcement of a metal-ceramic biocomposite	21
Caracterización estructural del cuasicristal $\text{Au}_{51}\text{Al}_{34}\text{Yb}_{15}$ , de su aproximante cristalino 1/1 y de sus fases nanoestructuradas	22
Colorings of Patterns Fixed by an Arbitrary Finite Index Subgroup of the Symmetry Group	23
Estudio local, microestructural y de estructura electrónica de la composición $\text{Fe}_{50}\text{Al}_{50}$ sintetizada por horno de arco	23
Influence of structural properties on magnetic properties in Fe/Ti superlattices with antiferromagnetic coupling	24
Magnetostructural coupling during the martensitic transformation in the $\text{Ni}_2\text{MnGa}$ Heusler alloy	25
Quantification of structural defects in hydroxyapatite doped with silver ions using the Rietveld method and their direct relationship to Methylene Blue photodegradation.	26
Resolving the chemical structure of [(7-chloroquinolin-4-yl) amino] acetophenones: A case of incorrect modeling and correction in Crystallography	27
Structural analysis by X-ray crystallography and biological studies of a thiosemicarbazone derived from [(7-chloroquinolin-4-yl) amino]-acetophenone	28
Structural characterization of new materials and archaeological ceramics	29
Structural effects of Palladium incorporation in thin films of $\text{Ni}_{50}\text{Mn}_{36}\text{Sn}_{14}$ by co-deposition	30

**ABSTRACT BOOK OF INTERNATIONAL SCHOOL ON FUNDAMENTAL CRYSTALLOGRAPHY:  
SEVENTH MATHCRYST SCHOOL IN LATIN AMERICA - PERU 2024**

Synthesis and characterization of gadolinium-doped cerium oxide nanoparticles	31
Synthesis and structural characterization of coordination compounds between 2- pyrazinecarboxylic acid and nickel(II): formation of molecular and polymeric compounds	32
Un estudio atómico del efecto de la composición sobre las propiedades estructurales y termodinámicas de las nanoaleaciones Al-Pd	33
Wide-Angle X-ray diffraction and Grazing Incidence X-ray diffraction study of ZnO nanostructured thin film	34
POSTER SESSION	35
PHOTOGRAPHS	37
VIDEOS	42
LIST OF PARTICIPANTS	43
SPONSORS	46

# **ABOUT THE SCHOOL**

The International School on Fundamental Crystallography, a series of educational schools in Latin America, commenced seventeen years ago at the University of Havana, Cuba, and has been hosted biannually in various countries across the region, including Havana, Cuba, Montevideo, Uruguay, Uberlândia, Brazil, La Plata, Argentina, and Bogota, Colombia. The school has served as an important space for the training of Latin American graduate students in the field of crystallography.

The VII edition of the school, set to take place in Lima, Peru, in 2020, was postponed due to the global COVID-19 pandemic. Consequently, at the request of the Peruvian academic community, the Commission on "Mathematical and Theoretical Crystallography" of the International Union of Crystallography (IUCr) granted the Faculty of Physical Sciences at the Universidad Nacional Mayor de San Marcos in Lima, Peru, the opportunity to organize the International School on Fundamental Crystallography: Seventh MaThCryst School in Latin America, from August 12 to 16, 2024.

The school, designed for students from the region, aims to bring together crystallographers from various countries and promote graduate studies in this scientific field. Since its first edition, the school has experienced steady growth in the number of participating Latin American professors and students, thanks to financial support from important institutions such as the IUCr, CLAF, and other regional universities. It is noteworthy that this event has already been recognized as an official school of the IUCr.

# **ORGANIZING COMMITTEES**

## **Chairperson**

Justiniano Quispe Marcatoma, Universidad Nacional Mayor de San Marcos

## **Local Committee**

Carlos Landauro Saenz, Universidad Nacional Mayor de San Marcos

Elvira Zeballos Velasquez, Universidad Nacional Mayor de San Marcos

Gladys Ocharan Velasquez, Universidad Nacional de San Agustín

Hector Loro Ramirez, Universidad Nacional de Ingeniería

Juan Carlos Gonzalez Gonzalez, Universidad Nacional Mayor de San Marcos

Lyda la Torre Riveros, Universidad Nacional de San Antonio de Abad del Cusco

Maria Luisa Ceron Loayza, Universidad Nacional Mayor de San Marcos

Maria Quintana Caceda, Universidad Nacional de Ingeniería

Silvia Espinoza Suarez, Universidad Nacional Mayor de San Marcos

Veronica Carranza Oropeza, Universidad Nacional Mayor de San Marcos

Victor Peña Rodríguez, Universidad Nacional Mayor de San Marcos

## **International Program Committee**

Mois I. Aroyo, University of the Basque Country, Spain

Massimo Nespolo, Université de Lorraine, France

Gemma de la Flor Martín, Karlsruhe Institute of Technology, Germany

María Cristina Nonato, University of São Paulo, Brazil

Leopoldo Suescun, Universidad de la República, Uruguay

Arbelio Penton-Madrigal, Universidad de la Habana, Cuba

## **REVIEW SYSTEM**

The abstracts were evaluated by the review committee, following the established guidelines in the editing process. The evaluation criteria included the structure and relevance of the research content. Finally, they were declared accepted for publication in the book of abstracts.

Reviewing committee:

- Dra. María Esther Quintana Caceda ([CTI-VITAE](#))
- Dr. Héctor Raúl Loro Ramírez ([CTI-VITAE](#))
- Dra. Silvia Marisel Espinoza Suarez ([CTI-VITAE](#))
- Dr. Justiniano Quispe Marcatoma ([CTI-VITAE](#))
- MSc. María Luisa Cerón Loayza ([CTI-VITAE](#))

## **GENDER EQUITY AND DIVERSITY POLICY**

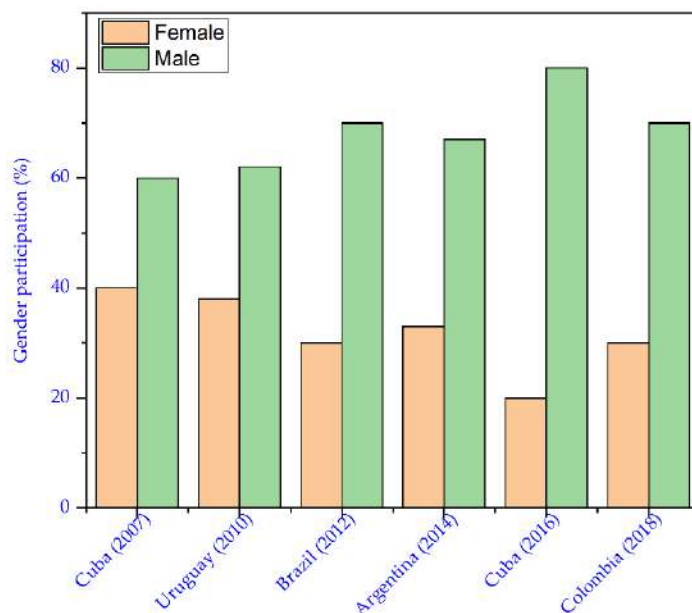
Herewith, we the organizers of International School on Fundamental Crystallography. Seventh MaThCryst School in Latin America endorse the IUCr GEDC Code of Conduct ([link](#)).

**Statement on Gender Balance at International School on Fundamental Crystallography. Seventh MaThCryst School in Latin America.**

The International School on Fundamental Crystallography. Seventh MaThCryst School in Latin America Organizing Committee fully supports and promotes gender equality in accordance with the IUCr policy <https://www.iucr.org/iucr/principles-and-policies/gender-balance>.

We will ensure gender equality in our committees (including the Organizing Committee itself), among our lecturers and participants and pay special attention to the gender balance in evaluating bursary applications.

Our gender statistics on female participation in the schools conducted are shown in the following graph. In this context and in accordance with IUCr policies and according to the observed behavior, in the present school we will emphasize female participation. For further information, our gender equity and diversity advisor is MSc. Maria Luisa Cerón Loayza (e-mail: [mceronl@unmsm.edu.pe](mailto:mceronl@unmsm.edu.pe)).



Further information can be found on the web site of IUCR's Gender Equity and Diversity Committee GEDC (<https://www.iucr.org/iucr/governance/advisory-committees/gedc>). This page contains a code of conduct, a GEDC conference speaker statement and a toolkit for conference organizers.

### **Scientific Freedom Policy Statement**

The Organizing Committee of International School on Fundamental Crystallography. Seventh MaThCryst School in Latin America shall observe the basic policy of non-discrimination and affirms the right and freedom of scientists to associate in international scientific activity without regard to such factors as ethnic origin, religion, citizenship, language, political stance, gender, sex or age, in accordance with the Statutes of the International Council for Science. At International School on Fundamental Crystallography. Seventh MaThCryst School in Latin America no barriers will exist which would prevent the participation of bona fide scientists.

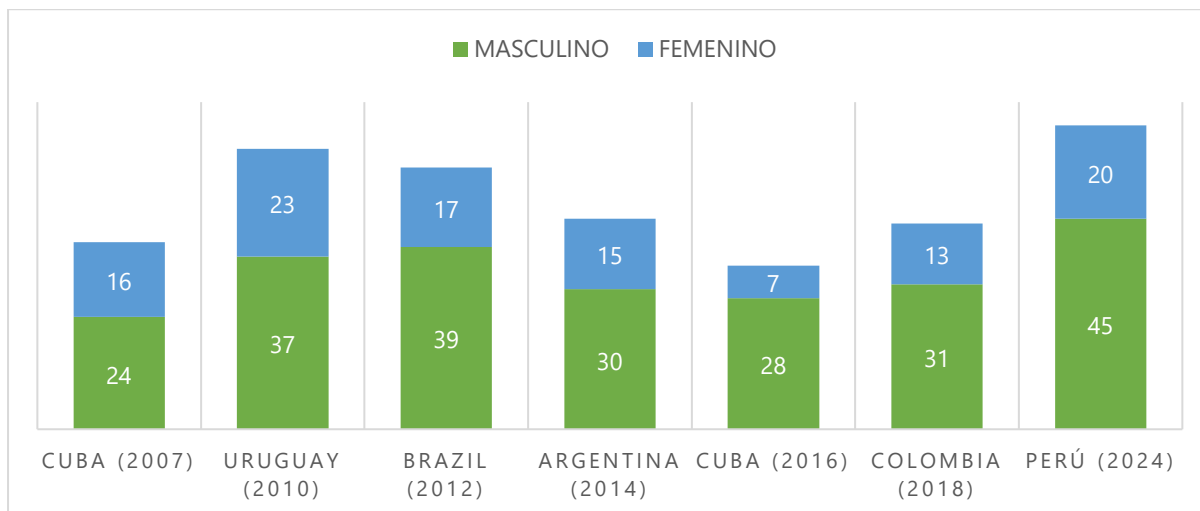
### **Diversity, Equality and Inclusion Statement**

We welcome all crystallographers and scientists working in related fields, regardless of their ethnic origin, race, citizenship, language, political views, gender, sex, sexual preferences, physical disabilities and age. We strive to create a culture of diversity, equality and inclusion.

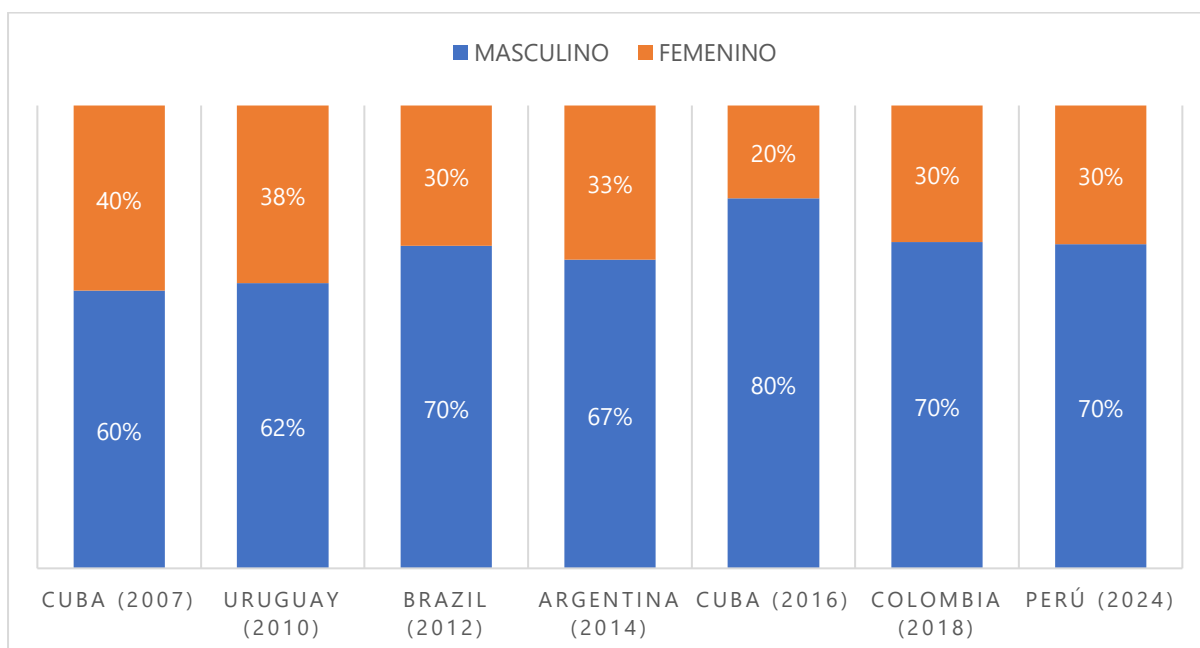


# DATA OF THIS EVENT

## NUMBER OF PARTICIPANTS



## GENDER OF THE PARTICIPANTS



## LECTURERS

### MASSIMO NESPOLO

Researcher in crystallography, magnetic resonance and modeling at the University of Lorraine, France.

Profiles: [ORCID](#) | [Scopus](#) | [HAL](#)



### MOIS ILIA AROYO

Researcher in mathematical crystallography at the University of the Basque Country, Spain..

Profiles: [ORCID](#) | [Scopus](#) | [Scholar](#)

### GEMMA DE LA FLOR MARTIN

Researcher in ferrous materials crystallography at the Karlsruhe Institute of Technology, Germany.

Profiles: [ORCID](#) | [Scopus](#) | [ReserchGate](#)



### ERNESTO ESTEVEZ-RAMS

Researcher in crystallographic calculations in reciprocal space at the University of Havana, Cuba. Profiles: [ORCID](#) |

[Scopus](#) | [ReserchGate](#)

### MARIA CRISTINA NONATO

Researcher in pharmaceutical sciences at the University of Sao Paulo, Brazil.

Profiles: [ORCID](#) | [Scopus](#) | [ResearchGate](#)



## TUTORS

### LEOPOLDO SUESCUN

Researcher in crystallography and materials chemistry at the Universidad de la República, Uruguay.

Profiles: [ORCID](#) | [Scopus](#) | [Scholar](#)



### MARIA LUISA CERÓN LOAYZA

Researcher specialized in the study and characterization of soils at the Universidad Nacional Mayor de San Marcos, Peru.

Profiles: [ORCID](#) | [Scopus](#) | [Scholar](#)



### ARBELIO PENTON-MADRIGAL

Researcher in crystallography and X-ray diffraction at the University of Havana, Cuba.

Profiles: [ORCID](#) | [Scopus](#) | [ReserchGate](#)



### LYDA LA TORRE RIVEROS

Researcher in electrochemistry and nanotechnology at the Universidad Nacional de Ingeniería, Peru.

Profiles: [ORCID](#) | [Scopus](#) | [ReserchGate](#)



## LANGUAGE

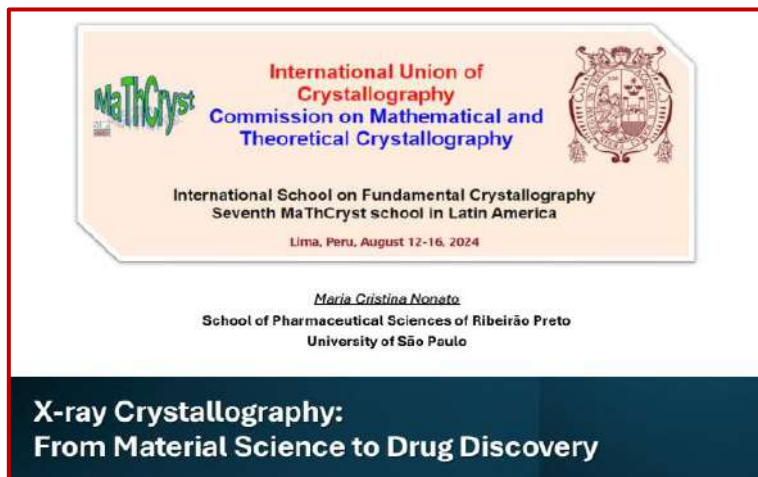
The official languages of the school are English and Spanish. Some classes will be taught in English, however the presence of Spanish-speaking tutors familiar with the classes beforehand will provide assistance to those who need it by translating or answering questions on the subject.

# PROGRAM FIRST DAY

## 12TH AUGUST 2024

### Opening lecture: María Cristina Nonato

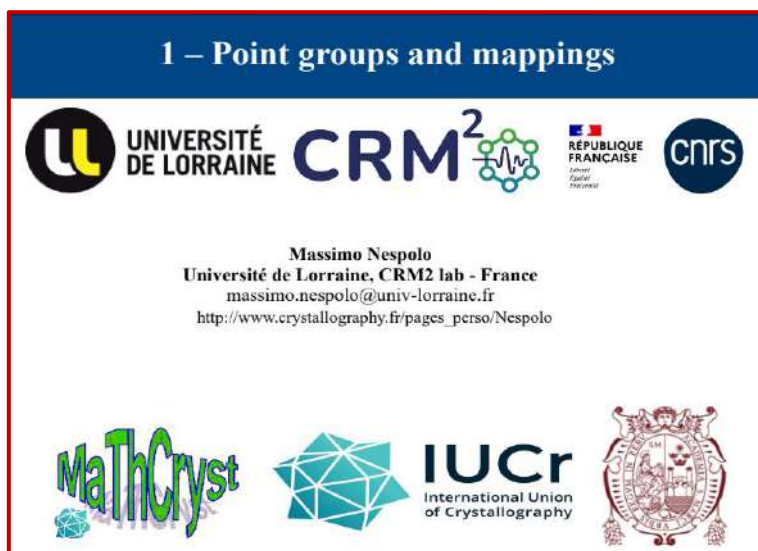
- X-ray crystallography: from material science to drug discovery



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### Morning lecture: Massimo Nespolo

- Symmetry groups and types of symmetry in direct space. Bravais lattices, conventional and non-conventional unit cells. Symmetry of lattices and symmetry directions. Hermann-Mauguin symbols for point groups. Symmetry of crystallographic patterns: holohedries and merohedries. Crystal families, lattice systems and crystal systems.



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**Afternoon lecture:** Massimo Nespolo y Mois Aroyo

- Miller indices. Morphological symmetry, forms and zone. Stereographic projection and its use for the derivation of crystallographic point groups.
- Basic properties of groups (group axioms, order, multiplication tables, etc.).
- Subgroups, index, coset decompositions, Lagrange theorem. Concept of isomorphism and homomorphism. Matrix-column presentation of symmetry operations. Symmetry elements: geometric elements and element sets. Geometric interpretation of the matrix-column presentation of the symmetry operations. Transformations of the coordinate systems: change of origin and orientation.

**CONTINUE READING**

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- Matrix-column presentation of symmetry operations. Symmetry elements: geometric elements and element sets. Geometric interpretation of the matrix-column presentation of the symmetry operations. Transformations of the coordinate systems: change of origin and orientation.

## LECTURE I

# CRYSTALLOGRAPHIC POINT GROUPS (basic facts)

**Contents:**  
Crystallographic point groups (basic facts).  
Matrix-column presentation of symmetry operations. Symmetry elements: geometric elements and element sets. Geometric interpretation of the matrix-column presentation of the symmetry operations.

Mois I. Aroyo  
Universidad del País Vasco, Bilbao, Spain



Universidad del País Vasco    Euzkai Herriko Unibertsitatea

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# PROGRAM SECOND DAY

## 13TH AUGUST 2024

**Morning lecture:** Mois Aroyo

- Group-subgroup relations (general considerations): index, coset decomposition and normal subgroups. Conjugation and normalizers; conjugate elements and conjugate subgroups; factor groups and homomorphism.
- Wyckoff positions for point group. Relations of Wyckoff positions for a group-subgroup pair. Supergroups of point groups.

### LECTURE 2

## GROUP-SUBGROUP RELATIONSHIPS

**Contents:**  
Group-subgroup relations of crystallographic point groups:  
Subgroups, index, coset decomposition and normal subgroups.  
General and special Wyckoff positions. Wyckoff positions  
splitting schemes.  
Group-supergroup relations. Normalizers.  
Conjugacy relationships: conjugate elements and conjugate  
subgroups. Group-subgroup graphs.

Mois I. Aroyo  
Universidad del Pais Vasco, Bilbao, Spain



Universidad del Pais Vasco Euskal Herriko Unibertsitatea

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**Afternoon lecture:** Massimo Nespolo

- Space groups - general introduction: periodic structure of the crystalline matter. Screw axes and glide planes.
- Orthogonal projections of space groups. Exercises on space-group diagrams from Volume A of the International Tables for Crystallography. General and special positions, site-symmetry groups.

2 - Bravais lattice and space groups



UNIVERSITÉ DE LORRAINE CRM<sup>2</sup> RÉPUBLIQUE FRANÇAISE cnrs

Massimo Nespolo  
Université de Lorraine, CRM2 lab - France  
massimo.nespolo@univ-lorraine.fr  
[http://www.crystallography.fr/pages\\_perso/Nespolo](http://www.crystallography.fr/pages_perso/Nespolo)



MaThCryst IUCr International Union of Crystallography

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## PROGRAM THIRD DAY

### 14TH AUGUST 2024

**Morning lecture:** Mois Aroyo

- Space groups and their description in International Tables for Crystallography, Vol. A. Algebraic determination of Wyckoff positions and site-symmetry groups.
- Computer databases and access tools to crystallographic symmetry data for space groups (International Tables for Crystallography, Volume A: Space-group symmetry): symmetry operations and their matrix-column presentation; geometric interpretation; general and special Wyckoff positions, site symmetry.

LECTURE 3a  
SPACE-GROUPS  
AND  
THEIR DESCRIPTIONS IN ITA

**Contents:**  
Crystal symmetry and its description by space groups. Hermann-Mauguin symbolism of space groups. Presentation of space-group symmetry operations in ITA. Space-group diagrams. Symmetry operations, geometric elements and symmetry elements. Unit cells and asymmetric units. General and special Wyckoff positions. Site symmetries. Coordinate transformations in crystallography.

Mois I. Aroyo  
Universidad del País Vasco, Bilbao, Spain



Universidad del País Vasco Euskal Herriko Unibertsitatea


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LECTURE 3b

# CO-ORDINATE TRANSFORMATIONS

**Contents:**  
Coordinate transformations in crystallography.

Mois I. Aroyo  
Universidad del Pais Vasco, Bilbao, Spain



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**Afternoon lecture:** Mois Aroyo


- Conventional and non-conventional descriptions of space groups; ITA settings.
- Group-subgroup relations between space groups: Subgroups of space groups: types of subgroups of space groups; Hermann theorem; maximal subgroups; series of isomorphic subgroups. Coset decomposition.

LECTURE 4a

# SPACE-GROUP SYMMETRY RELATIONS

**Contents:**  
Maximal subgroups of space groups:  $t$ - and  $k$ -subgroups.  
General subgroups of space groups; group-subgroup index and its factorization.  
Hermann theorem and Hermann group for a general group-subgroup pair.  
Wyckoff-position splitting schemes.

Mois I. Aroyo  
Universidad del Pais Vasco, Bilbao, Spain



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## LECTURE 4b

# SPACE-GROUPS SYMMETRY RELATIONS APPLICATIONS

**Contents:**  
Domain-structure analysis in phase-transition problems (initial steps)  
Orientational and anti-phase domain states crystallography.  
Supergroups of space groups  
Normalizers of space groups

Mois I. Aroyo  
Universidad del País Vasco, Bilbao, Spain



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## PROGRAM FOURTH DAY

### 15TH AUGUST 2024


**Morning lecture:** Leopoldo Suescun, Maria Cristina Nonato, Arbelio Penton-Madriral, Ernesto Estevez Rams.

- Reciprocal space
- Crystallographic calculations in reciprocal space
- Introduction to diffraction
- Diffraction symmetry: Laue classes, Friedel's law, resonant scattering.
- Integral, zonal and serial reflection conditions and their use to determine the space-group type. Special reflection conditions.

**ABSTRACT BOOK OF INTERNATIONAL SCHOOL ON FUNDAMENTAL CRYSTALLOGRAPHY:  
SEVENTH MATHCRYST SCHOOL IN LATIN AMERICA - PERU 2024**



**International Union of  
Crystallography**  
**Commission on Mathematical and  
Theoretical Crystallography**




**International School on Fundamental Crystallography  
Seventh MaThCryst school in Latin America**

Lima, Peru, August 12-16, 2024

- Reciprocal space
- Crystallographic calculations in reciprocal space
- Introduction to diffraction
- Diffraction symmetry: Laue classes, Friedel's law, resonant scattering.
- Integral, zonal and serial reflection conditions and their use to determine the space-group type. Special reflection conditions.

International Table of Cryst. (ITC), Vol A and B.  
Fundamentals of Cryst. by C. Giacovazzo, IUCr, Oxford Uni. Press, 4<sup>th</sup> Edit. 2000

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**INTRODUCTION TO X-RAY  
DIFFRACTION**

LCP-RP  
LABORATÓRIO DE CRISTALOGRAFIA DE PROTEÍNAS

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**crystmat-lab**



**UDELAR  
FACULTAD DE  
QUÍMICA**



**UNIVERSIDAD  
DE LA REPÚBLICA  
URUGUAY**

***Systematic Absences and Space Group  
Determination***

Leopoldo Suescun  
Laboratorio de Cristalografía Química del Estado Sólido y Materiales,  
Facultad de Química, Universidad de la República,  
Montevideo, Uruguay.  
leopoldo@fq.edu.uy

Agosto 15, 2024

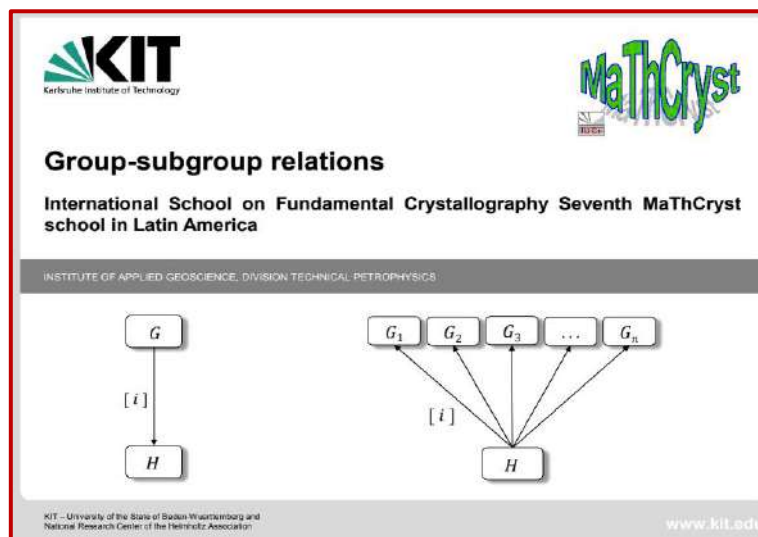
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# PROGRAM FIFTH DAY

## 16TH AUGUST 2024

**Morning lecture:** Gemma de la Flor Martín

- Maximal subgroups data and related computer applications: (i) Introduction and use of the databases of the IT-Online server and the Bilbao Crystallographic server of maximal subgroups, series of isomorphic subgroups and minimal supergroups; (ii) General group-subgroup relations between space groups: computer programs on the IT-Online server and the Bilbao Crystallographic Server.
- Relations of Wyckoff positions for a group-subgroup pair. Supergroups of space groups.

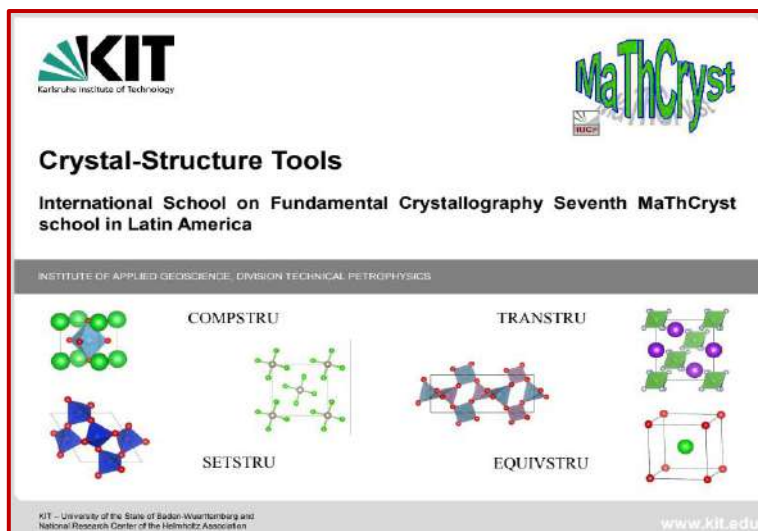


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**Afternoon lecture:** Gemma de la Flor Martín

- Crystal-structure descriptions I. Basis transformations and crystal-structure descriptions; structure descriptions compatible with symmetry reduction (the program TRANSTRU). Descriptions of crystal structures with respect to different ITA settings of the space groups (the program SETSTRU). Equivalent crystal structure descriptions (the programs EQUIVSTRU and COMPSTRU).
- Crystal-structure relations. Group-subgroup relations between space groups and the construction of structure family trees (Baernighausen trees (the program STRUCTURE RELATIONS)).

**ABSTRACT BOOK OF INTERNATIONAL SCHOOL ON FUNDAMENTAL CRYSTALLOGRAPHY:  
SEVENTH MATHCRYST SCHOOL IN LATIN AMERICA - PERU 2024**



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**Closing lecture:** María Cristina Nonato

Fragment screening by X-ray crystallography, an important tool to develop new therapies against infectious diseases.



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# A Parallelizable X-Ray Diffraction Pattern Simulation for Fast Rietveld Refinement

Miguel Angel Arbelaez Llano<sup>1\*</sup>, Jairo Roa-Rojas, David Arsenio Landinez Tellez

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Rietveld refinement, a method used to determine crystal structures from Powder X-Ray Diffraction (PXRD) patterns, is one of the most successful algorithms in crystallography. Though technological advances in data collection and analysis techniques have allowed for its application to bigger and more complex molecules, the algorithm's computational cost remains high, and the successful determination of macromolecular structures usually requires the combination of data from various sources [1]. To address this issue, we present a fast and easily parallelizable PXRD pattern simulation algorithm. By applying vectorization techniques and expressing the calculation of structure factors entirely in terms of matrix operations, it is possible to efficiently distribute the necessary calculations for Rietveld refinement even when the unit cell contains a large number of atoms, where the current approach by Zeitler and Toby struggles [2]. The program's precision was verified by comparing its predictions to multiple entries in the Crystallography Open Database [3], obtaining a Bragg R factor  $RB < 0.05$  for all analyzed compounds. A Hessian Rietveld refinement algorithm was implemented and the convergence of structural parameters for a Ba<sub>2</sub>SbSmO<sub>6</sub> sample towards their literature values was reached in only 6 iterations ( $R_p=0.076$ ). These results indicate the feasibility of updating Rietveld refinement algorithms to make more efficient use of modern high-performance computing infrastructure and solve more complex molecules at high resolution.

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## Keywords

Rietveld Refinement, Powder X-Ray Diffraction, Parallel Processing, High-Performance Computing

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# Atomic structure of the $i\text{-Al}_64\text{Cu}_{23}\text{Fe}_{13}$ aperiodic crystal and its application as a mechanical reinforcement of a metal-ceramic biocomposite

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Aperiodic crystals or quasicrystals (QCs), discovered in 1984 by Daniel Schechtman, are structures that lack translational symmetry, but have long-range ordering [1]. These characteristics give them interesting properties as a thermal insulator, low coefficient of friction and unusual paramagnetism [2]. On the other hand, hydroxyapatite (HAp) -based compounds are commonly used as bone prostheses or dental resin filler particles due to their similarity to the inorganic component of the human hard tissues. However, these materials are fragile under mechanical loads and impacts. Thus, by incorporating metal compounds such as QCs, which possess greater ductility, it is possible to improve the mechanical performance and obtain a more durable biomaterial. In the present work, the quasicrystal  $\text{Al}_64\text{Cu}_{23}\text{Fe}_{13}$  with icosahedral symmetry was synthesized by arc furnace and it was characterized by X-ray diffraction, scanning electron microscopy, vibrating sample magnetometry and Vickers microhardness. Then, it was incorporated, in different concentrations, into a metal-ceramic biocomposite based on HAp (matrix). The mechanical properties of the resulting composites were determined through mechanical compression tests. Additionally, cytotoxicity assays were performed on two cell lines to evaluate the potential biomedical application of these biocomposites. The results showed the structural quality of the quasicrystal obtained by arc furnace evidenced by sharp peaks in its diffractogram and grains with pentagonal faces in its micrographs (icosahedral symmetry). Likewise, an increase in Young's modulus and in the maximum deformation of the biocomposites was observed as the quasicrystal was added. Finally, none of the biocomposites exhibited cytotoxicity against the tested cell lines, reaffirming their potential use in biomedical applications [3].

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## Keywords

Quasicrystal, Hydroxyapatite, Biocomposite

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## Caracterización estructural del cuasicristal Au<sub>51</sub>Al<sub>34</sub>Yb<sub>15</sub>, de su aproximante cristalino 1/1 y de sus fases nanoestructuradas

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En este trabajo se realizó la caracterización estructural del sistema Au-Al-Yb en sus fases periódica y cuasiperiódica sintetizadas mediante la técnica de horno de arco voltaico. La fase aperiódica fue indexada utilizando el método de corte y proyección, cuyo patrón de difracción de rayos X revela una estructura icosaédrica de tipo P con un parámetro de red 6- dimensional (a<sub>6D</sub>) de 7.45 nm. La fase periódica fue analizada mediante el refinamiento Rietveld, revelando una estructura cúbica con grupo espacial Im $\bar{3}$  y un parámetro de 14.54 nm, identificada como el aproximante 1/1 de la fase cuasicristalina. La nanoestructuración mediante molienda mecánica se llevó a cabo en un molino de bolas planetario, resultando en una reducción del tamaño de grano promedio tras un tiempo de molienda de 10 horas tanto en el cuasicristal como en el aproximante cristalino. En el cuasicristal, el tamaño de grano disminuyó de 64.13 nm a 47.33 nm, mientras que en el aproximante cristalino se redujo de 108.4 nm a 37.11 nm. Esta reducción en el tamaño de grano afecta las propiedades microestructurales, provocando una alteración en las propiedades físicas del material. Estos cambios indican la efectividad de la nanoestructuración en modificar las características internas de ambas fases, lo cual influye directamente en sus correspondientes propiedades físicas.

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### Keywords

Cuasicristales, Aproximantes Cristalinos, Difracción De Rayos X, Nnoestructuración

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## Colorings of Patterns Fixed by an Arbitrary Finite Index Subgroup of the Symmetry Group

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In this research project, we establish a framework that characterizes the colorings of a pattern fixed by an arbitrarily chosen finite index subgroup of the pattern's symmetry group. This framework is applied to the sphalerite structure to enumerate all colorings fixed by two different subgroups of the symmetry group. These colorings are used to perform ordered substitution on the atoms in the sphalerite structure and exhibit some of the well-known derived structures (e.g. chalcopyrite, stannite). Some results involving equivalences of colorings fixed by the chosen subgroup are also developed.

### Keywords

Color Symmetry, Equivalent Colorings, Sphalerite, Derived Structures

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## Estudio local, microestructural y de estructura electrónica de la composición Fe<sub>50</sub>Al<sub>50</sub> sintetizada por horno de arco

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Las aleaciones metálicas Fe - Al en las regiones ricas en hierro son de importancia debido a sus interesantes propiedades magnéticas presentes en su estado nanocristalino en el cual son usados en dispositivos de memoria magnética y en sensores magnéticos, mientras que para regiones ricas en aluminio estas aleaciones son usadas en la industria automotriz, espacial y marítima a causa de su baja densidad y excelente resistencia a la corrosión. En la composición Fe<sub>50</sub>Al<sub>50</sub> fue sintetizado por la técnica de horno de arco y luego tratado térmicamente a 6000C. Los difractogramas de rayos X (DRX) y espectroscopia Mòssbauer (EM) muestra la formación del intermetálico FeAl, la solución sólida Fe(Al) y un remanente de Fe a temperatura ambiente. Quedando solo el intermetálico FeAl y la solución sólida Fe(Al) luego del tratamiento térmico. Los cálculos de estructura electrónica basados en la aproximación de la densidad Local utilizando la teoría de la densidad funcional DFT a partir de los resultados de DRX EM muestran que el intermetálico FeAl es metálico [1, 2].



## **Keywords**

Espectroscopia Mössbauer, Difracción De Rayos X, Horno De Arco, Teoría De La Densidad Funcional.

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**N° 6**

# **Influence of structural properties on magnetic properties in Fe/Ti superlattices with antiferromagnetic coupling**

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Multilayer-based systems exhibiting synthetic antiferromagnetic coupling (SAF) are the subject of intensive investigation due to their zero net magnetization, which avoids the formation of stray fields. This makes these systems suitable for applications in the next generation of electronic and spintronic sensors [1-3]. SAFs are composed of two ferromagnetic (FM) layers spaced by a non-magnetic (NM) layer. In such multilayers, the magnetization of the ferromagnetic layers are coupled to each other through interlayer exchange interaction, which is mediated by the electrons in the spacer layer. This type of interaction is described by the model proposed by Ruderman-Kittel-Kittel-Kasuya-Yosida (RKKY) for magnetic impurities. This interaction oscillates with the thickness of the spacer (non-magnetic layer). Consequently, by varying the spacer thickness, an antiparallel alignment between the magnetization of the ferromagnetic layers can be achieved, which is indicative of an antiferromagnetic coupling (AFM) or a parallel alignment, which is indicative of a ferromagnetic coupling (FM) [3]. In addition, other factors may influence the magnitude of the interlayer exchange constant. These include interface effects, surface roughness, interdiffusion of adjacent materials, generation of magnetically dead layers, crystalline defects and lattice parameter mismatch between adjacent layers [1]. In this context, the structural and magnetic properties of antiferromagnetically coupled Fe/Ti superlattices were studied. The structural characterization was carried out by X-ray diffraction, which enabled the identification of the crystalline phase present and the preferred crystallographic orientation. Low-angle X-ray reflectivity (XRR) was used to determine the thickness of the superlattices. A high-resolution transmission electron microscope (HRTEM) was employed for structural and morphological analysis; from the electron diffraction pattern crystalline phase is identify. In addition, the static and dynamic magnetic properties were investigated by superconducting quantum interference device magnetometry and vector network analyzer ferromagnetic resonance, respectively. The interlayer exchange constant was determined from the static magnetization analysis, revealing a weak antiferromagnetic coupling that is associated with structural and morphological factors affecting its magnetic response. Furthermore, a macrospin model was employed to simulate the static magnetic response, thereby enabling the acquisition of diverse magnetic parameters, including the interlayer exchange coupling constant, which considers the biquadratic coupling, due to the roughness of the interfaces.

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## Keywords

Synthetic Antiferromagnet, Interlayer Exchange Coupling, Structural Characterization, Magnetic Characterization

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**N° 7**

# **Magnetostructural coupling during the martensitic transformation in the Ni<sub>2</sub>MnGa Heusler alloy**

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The Ni<sub>2</sub>MnGa Heusler alloy is a functional material that presents interesting properties, including shape memory effects and magnetocaloric effects. These phenomena are associated with magnetostructural phase transitions [1]: a martensitic transformation (from a cubic L21 structure at high temperatures to a tetragonal L10 structure at low temperatures) coupled to a magnetic phase transition (from paramagnetic to ferromagnetic, upon cooling of the system). Under some conditions, it is possible the appearance of intermediate structural phases, the so-called premartensitic phases [2]. These phases strongly modify the magnetostructural properties of Ni<sub>2</sub>MnGa. If we consider that these phases are made of two interacting subsystems, we expect some correlation between them. Furthermore, such correlations should change during the phase transitions, controlled by the variation of the temperature. In this work, the entropy of the total system (using the Montecarlo-Metropolis method and the mean field approximation) and of the subsystems (using the Gibbs definition) are calculated to study the correlation changes occurring in the system during the phase transition. In both cases, we use a Hamiltonian model that has three contributions [3]: the structural contribution (where the Blume-Emery-Griffiths model was used to describe the elastic variables associated with the local deformation of the lattice), the magnetic contribution (where the Potts model is used to describe the spins) and the contribution of the interaction among the magnetic and elastic variables. The preliminary results show that it is possible to describe the experimental findings using this simplified model which allow us to describe the complexity of the structural and magnetic changes occurring during the phase transformation.

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## Keywords

Martensitic Transformation, Blume–Emery–Griffiths, Monte Carlo Metropolis

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**N° 8**

# **Quantification of structural defects in hydroxyapatite doped with silver ions using the Rietveld method and their direct relationship to Methylene Blue photodegradation.**

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Hydroxyapatite (Ca<sub>5</sub>(PO<sub>4</sub>)<sub>3</sub>OH), a mineral found in human bone and dental tissues, has garnered interest due to its biomimetic properties and its ability to host metal ions such as silver (Ag<sup>+1</sup>), copper (Cu<sup>+2</sup>), zinc (Zn<sup>+2</sup>), cobalt (Co<sup>+2</sup>), iron (Fe<sup>+3</sup>), strontium (Sr<sup>+2</sup>), among others [1]. From a structural perspective, hydroxyapatite exhibits a hexagonal crystal structure with space group P6<sub>3</sub>/m, characterized by its network of calcium, phosphate, and hydroxyl ions [2]. In recent years, hydroxyapatite has also been used in environmental remediation, such as in the degradation of dyes and colorants, prompting research to enhance its attributes by modifying its crystal structure through doping with different metal ions like copper (Cu<sup>+2</sup>), zinc (Zn<sup>+2</sup>), and silver (Ag<sup>+1</sup>) [3]. The substitutional addition of silver ions (Ag<sup>+1</sup>) at the Ca (I) and Ca (II) sites introduces interesting challenges due to their size, electronic configuration, and affinity for certain crystal sites within the hydroxyapatite matrix. The Rietveld method, an advanced technique for refining crystal structures based on fitting X-ray diffraction patterns, is employed to analyze how the crystal structure varies when silver ions are introduced into hydroxyapatite. This approach allows not only for the quantification of the amount of incorporated silver but also for mapping changes in lattice parameters, atomic positions, and site occupancies. This structural study aims to understand how silver ions are incorporated into the crystal structure of hydroxyapatite and how this incorporation affects the physical and chemical properties of the resulting material in the photodegradation of Methylene Blue (MB).

### Keywords

Hydroxyapatite, Silver-Dopping, Rietveld Method, Microstructure, Methylene Blue.

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N° 9

## Resolving the chemical structure of [(7-chloroquinolin-4-yl) amino] acetophenones: A case of incorrect modeling and correction in Crystallography

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In materials science and chemistry, proper characterization of a material or compound is crucial to understanding its chemical nature and the three-dimensional distribution or conformation of the atoms or molecules comprising it. Crystallography and X-ray diffraction techniques in this field enable the determination of the crystalline structure of solid materials, thereby establishing their chemical identity [2]. Occasionally, incorrect structural models can yield seemingly reliable parameters during structural refinement [3]. Therefore, the determined structure must undergo thorough analysis, ensuring the model aligns with chemical principles. In this contribution, we present a simple example illustrating the initial incorrect modeling of the chemical composition of 1-{3-[(7-chloroquinolin-4-yl) amino]phenyl}ethan-1-one, and the correct approach for successfully resolving the structure [1]. The compound crystallizes in a triclinic P-1 system with parameters  $a = 8.4271(9) \text{ \AA}$ ,  $b = 8.5106(10) \text{ \AA}$ ,  $c = 12.4209(13) \text{ \AA}$ ,  $\alpha = 79.950(9)$ ,  $\beta = 77.911(9)$ ,  $\gamma = 67.81(1)$ ,  $V = 802.06(16) \text{ \AA}^3$  and  $Z = 2$ . Several yellow plate-like crystals were selected for room-temperature data recording using molybdenum irradiation. The reduction and integration of the data were consistent concerning the same molecular formula structure  $C_{17}H_{14}ClN_2O \cdot Cl$  with positional disorder in the ethanone fragment.

### Keywords

Quinoline, Refinement, Crystallographic Model, Structure.

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## Structural analysis by X-ray crystallography and biological studies of a thiosemicarbazone derived from [(7-chloroquinolin-4-yl) amino]-acetophenone

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This study presents the synthesis, characterization, in silico and in vitro biological evaluation of a thiosemicarbazone derived from [(7-chloroquinolin-4-yl)amino]-acetophenone. The structure of the compound was determined by single-crystal X-ray diffraction using Mo-K $\alpha$  radiation ( $\lambda = 0.71069 \text{ \AA}$ ) alongside other techniques. The compound crystallizes in a triclinic P-1 (No.2) system with final cell constants of  $a = 9.1204(7) \text{ \AA}$ ,  $b = 10.8893(9) \text{ \AA}$ ,  $c = 11.1300(9) \text{ \AA}$ ,  $\alpha = 85.013(2)^\circ$ ,  $\beta = 72.957(2)^\circ$ ,  $\gamma = 67.152(2)^\circ$ ,  $V = 973.46(14) \text{ \AA}^3$  and  $Z = 2$  ( $R_{int} = 3.74\%$ ,  $R_{sig} = 4.08\%$ ,  $R_1 = 4.60\%$ ,  $wR_2 = 13.35\%$ ,  $S = 1.05$ ). The reduction and integration of the data were consistent with the molecular formula  $C_{18}H_{19}ClN_5S_2O_1$ , revealing electronic density consistent with an S(2) environment, possibly at the H<sub>2</sub>S formation as a byproduct (CCDC 1413401). Its inhibitory activity against the chloroquine-resistant strain (W2) of *Plasmodium falciparum* was assessed, along with its effects on hemozoin ( $\beta$ -hematin) formation and cysteine protease falcipain-2. The results indicate significant potency against the parasite, albeit showing reduced activity towards hemozoin formation and falcipain-2 inhibition. [1] In silico studies confirm that the effective p-p interactions appear to determine the activity of a compound in inhibiting hemozoin crystal growth.

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<http://dx.doi.org/10.17807/orbital.v9i4.1001>

### Keywords

Thiosemicarbazone, Crystal Structure, Antiplasmodial Activity

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## Structural characterization of new materials and archaeological ceramics

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Our laboratory provides state-of-the-art tools for structural characterization through X-ray diffraction (XRD) and elemental composition analysis via X-ray fluorescence (XRF). These techniques are crucial for detailed material analysis, enabling the assessment of parameters such as crystallite size, internal stresses, crystallinity percentage, and the identification of phases in ceramic materials. MATERIALS AND METHODS. To obtain materials for dosimetric applications, we use sol-gel, precipitation, combustion, hydrothermal, solid-state reaction, and other methods. In the case of dating, to obtain quartz, we use chemical treatments.

RESULTS AND DISCUSSION.

- A) XRD patterns of phosphor  $\text{Ca}_2\text{Al}_2\text{SiO}_7$  doped with x mol% Ce (x = 0.00, 0.10, 0.25, 0.50, 0.75, 1.00, and 2.00)
- B) Rietveld refinement results of the XRD pattern
- C) XRD pattern of the Churajon sample. Two crystalline phases  $\text{SiO}_2$  and  $\text{K}(\text{AlSi}_3)\text{O}_8$  were identified with the files 01-085-0794 and 01-075-1190 PDF-2

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### Keywords

Dosimetric Applications, Hydrothermal, Solid-State Reaction

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## Structural effects of Palladium incorporation in thin films of Ni<sub>50</sub>Mn<sub>36</sub>Sn<sub>14</sub> by co-deposition

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Heusler compounds exhibit a wide range of technologically interesting physical properties, but these are highly sensitive to structural defects. Even with an ordered crystal structure, chemical disorder can negatively impact their properties. Ideally, an X<sub>2</sub>YZ Heusler compound crystallizes in a cubic space group Fm $\bar{3}$ m (number 225), where X, Y, and Z atoms occupy specific Wyckoff positions. This L21 structure can be seen as four interpenetrating fcc sublattices, two of which are equally occupied by X. Chemical disorder in the L21 structure can be classified by atom swapping within the unit cell: random swapping between X/Y or X/Z atoms produces a B32a disorder; swapping between X/Y atoms produces a D03 disorder; swapping between Y/Z atoms produces a B2 disorder; and swapping between all atoms produces an A2 disorder.

To investigate chemical disorder, various experimental techniques are available, with x-ray diffraction (XRD) being one of the most common. XRD patterns can help characterize chemical disorder because each type is associated with the absence of certain superstructure reflections, such as (111), (200), and (311).

Typically, the appearance of these reflections indicates a perfect L21 structure. However, D03 disorders or inverse Heusler compounds can also exhibit these reflections, necessitating a quantitative study of intensities to differentiate between them. In Heusler compounds where the atomic scattering factors of X and Y are similar, conventional XRD analysis is insufficient, requiring high-resolution techniques.

To understand the effect of Pd atom incorporation in Ni-Mn-Sn thin films, grazing incidence XRD was used to study the crystal structure and chemical disorder. Samples of Ni-Mn-Sn and Ni-Mn-Sn-Pd thin films were grown at different temperatures. The incorporation of Pd atoms clearly impact in lattice parameter yielding larger lattice parameter. The lattice parameter of the sample grown at room temperature was the largest of the samples. For samples grown at high temperatures, the parameter was reduced. Finally, the types of disorder were characterized by the absence of reflection peaks.

### Keywords

Heusler Compounds, Thin Films, X-Ray Diffraction, Chemical Disorder

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## Synthesis and characterization of gadolinium-doped cerium oxide nanoparticles

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A sample of gadolinium-doped cerium oxide (GDC) was prepared by a co-precipitation method of sodium hydroxide, cerium nitrate, and gadolinium nitrate. The material was characterized by two X-ray techniques to evaluate the structural properties: 1. X-ray diffraction (XRD) finding that the powders present cubic phase, space group, unit cell parameters  $a = 5.4155 \pm 0.0003 \text{ \AA}$ ,  $V = 158.82 \text{ \AA}^3$ , and crystallite size of about 13 nm. 2. X-ray photoelectron spectroscopy (XPS), where the spectra recorded for the Ce3d [Ce3d3/2 (918.0 eV) and Ce3d5/2 (884.0 eV)], O1s (530.6 eV), and Gd4d [Gd4d3/2 (153.8 eV) and Gd4d5/2 (142.5 eV)] core levels of GDC powder.

The Ce3d spectra show a multiplet structure, corresponding to three final states with 3d94f0, 3d94f1, and 3d94f2L configurations for 3d3/2 and 3d5/2. The 3d94f2L configuration is caused by the charge transfer from the O2p to Ce4f orbital due to a lowered energy level caused by a strong electrostatic core-hole interaction. A peak confirms Ce(IV) form at 918 eV, absent in the Ce(III) spectrum. [1-3] However, Rietveld refinements of XRD data revealed a high Debye-Waller factor, suggesting that Na<sup>+</sup> ions could be incorporated into the crystal lattice. This will be subject of additional studies.

### Keywords

Ceria, Gadolinium-Doping, Nanoparticles

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## Synthesis and structural characterization of coordination compounds between 2- pyrazinecarboxylic acid and nickel(II): formation of molecular and polymeric compounds

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The synthesis of coordination compounds has gained great interest not only because of their structural diversity and the different topologies they may present, but also because of their possible applications in fluorescence, electricity, magnetism and their use in homogeneous catalysis. The synthesis routes are crucial for obtaining new structures that present the aforementioned properties. In this sense, the solvothermal synthesis and characterization of two Ni(II) coordination compounds was carried out using infrared, Raman, powder and single crystal X-rays diffraction, thermogravimetric analysis, differential scanning calorimetry, elemental analysis and scanning electron microscopy techniques. The single crystal X-rays results confirmed the obtaining of a molecular compound that crystallizes in a monoclinic P21/c space group while the second compound corresponds to a coordination polymer that crystallizes in an orthorhombic P212121 space group. It is important to note that the hydrolysis of the precursor ligand, 2-pyrazinecarboxamide, was promoted by the metal and the solvothermal synthesis conditions, leading to the formation of two coordination compounds between Ni(II) and the in situ generated 2-pyrazinecarboxylic acid. The results of the thermogravimetric analysis show that the decomposition of the two coordination compounds occurs around 343 °C. Furthermore, theoretical analyses of the solid-state interaction energies were carried out, which showed that the electrostatic energy prevails over the dispersion energy which occurs in interactions between heteroatoms; these O...H interactions are responsible for crystal growth since they control the molecular packing and generate different topologies.

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## Un estudio atomístico del efecto de la composición sobre las propiedades estructurales y termodinámicas de las nanoaleaciones Al-Pd

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Las nanopartículas intermetálicas (NP) son de gran interés debido a las propiedades únicas derivadas de su composición y estructura, como una mayor estabilidad térmica y el potencial para mejorar la actividad catalítica a través de la variación de la estequiometría y el tamaño de las NP [1]. En particular, las NP intermetálicas de Al-Pd tienen diversas aplicaciones, desde en el ámbito biomédico, gracias a su ultrabaja susceptibilidad magnética, hasta las energías renovables, debido al incremento de la superficie de reacción y que proporciona una excelente selectividad en procesos de catálisis.

Sin embargo, este sistema ha sido bastante controversial debido a la complejidad de su diagrama de fases y sus límites [3]. El objetivo de este trabajo es calcular las propiedades térmicas y estructurales de NPs de Al-Pd para varios tamaños y concentraciones que van desde el 10% al 90% de Al, utilizando simulación atomística mediante el método de dinámica molecular.

Se parte de una distribución aleatoria de átomos de Al y Pd en una NP con una estructura inicial FCC. Luego, se simulan los procesos de calentamiento y enfriamiento del sistema utilizando el paquete LAMMPS con el potencial interatómico del método del átomo embebido modificado (MEAM). Posteriormente, para la caracterización estructural se utilizaron diversas herramientas del software OVITO, como la técnica de análisis de vecinos comunes (CNA) y la función de distribución radial (RDF). Los resultados preliminares obtenidos muestran, a partir del cálculo de la capacidad calorífica, para cada composición, la relación directamente proporcional de la temperatura de fusión con el tamaño de las nanopartículas, el cual tiende al valor macroscópico.

Además, para la nanoaleación de AlPd, se ha formado un compuesto intermetálico ordenado, donde cada átomo de Al está rodeado por átomos de Pd y viceversa, cuyas características estructurales como el parámetro de red y la estructura cristalina calculada teóricamente concuerdan con los resultados experimentales. Por otro lado, la curva de histéresis térmica para cada composición y tamaño está bien definida sólo después del recalentamiento, lo que indica que la estructura cristalina obtenida después del proceso enfriamiento es propia del sistema.

Finalmente, parte de la caracterización del sistema incluye el análisis de las gráficas obtenidas a partir de los datos del índice de Lindemann, el desplazamiento cuadrático medio (MSD) y el radio de giro proporcionados por LAMMPS. Así como el cálculo de la dispersión de fonones, que permitió determinar la estabilidad dinámica de las fases de las NPs a simular.

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### Keywords

Dinámica Molecular, Nanopartículas Binarias, Aluminio - Paladio, Caracterización Estructural

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**N° 16**

## **Wide-Angle X-ray diffraction and Grazing Incidence X-ray diffraction study of ZnO nanostructured thin film**

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Reactive magnetron sputtering is one of the most popular techniques to grow thin films in science and technology due to the high quality of the thin films obtained, the possibility of working on large substrates, and the high ratio of deposition obtained. We studied the surface structure of ZnO nanostructured thin films grown on a glass substrate by wide-angle X-ray diffraction and grazing incidence X-ray diffraction [1]. Both experimental techniques are surface sensitive for interrogating ZnO nanostructured thin films using small incidence angles.

### Keywords

Zno Oxide Thin Films, Nanocolumns, Reactive Magnetron Sputtering, WAXRD, GIXRD

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## POSTER SESSION



Award for the best poster of the session



First place, Allan O. Junio, and second place, Yonathan J. Parra.



## COLORINGS OF PATTERNS FIXED BY AN ARBITRARY FINITE-INDEX SUBGROUP OF THE SYMMETRY GROUP

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### Introduction

Vaughan and Corkhill [2017] discussed metal sulfides and the relationships between parent crystal structures and their derived structures. One such relationship is called *ordered substitution*, a process of systematically replacing atoms in the parent structure to derive a new structure.

In this research, we use color symmetry to perform ordered substitution. In color symmetry, elements of symmetric objects and structures are colored to study these structures, their symmetry groups and subgroups of these symmetry groups. In particular, we take inspiration from some of the ideas in Walo and Felix [2011].

### Objectives

- characterize the colorings of a pattern fixed by an arbitrarily chosen finite-index subgroup of the pattern's symmetry group
- develop a framework for constructing such colorings according to the characterization

### Main Results and Coloring Framework

Let  $X$  be a set with symmetry group  $G$ , and let  $K < G$ .

**Proposition 1** A coloring  $\mathcal{P} = \{P_1, P_2, \dots, P_n\}$  of  $X$  is fixed by  $K$  if and only if each  $P_i$  is a union of  $K$ -orbits of elements of  $X$ .

**Lemma 2** If  $a \in N_G K$ , then  $a$  permutes the  $K$ -orbits.

**Lemma 3** If  $a \in G$  permutes the  $K$ -orbits, then  $aKx = Kax$  for all  $x \in X$ .

**Theorem 4** Let  $x_i \in X$ ,  $X_i = Gx_i \subseteq X$ , and  $K \leq G$  such that  $X_i = Kq_i \cup Kq_2 \cup \dots \cup Kq_n$ , with  $\text{Stab}_G q_i \leq K$  for each  $i$ . Then, the subgroup of  $G$  that permutes the  $K$ -orbits is precisely  $N_G K$ .

**Theorem 5** The number of inequivalent colorings of  $X$  fixed by  $K$  is at most the number of orbits of  $G$  under the action of  $N_G K$ , where  $G$  is the set of colorings constructed according to proposition 1. If each  $K$ -orbit has an element whose stabilizer is a subgroup of  $K$ , then the number of inequivalent colorings of  $X$  fixed by  $K$  is precisely the number of orbits of  $G$  under the action of  $N_G K$ .

#### COLORING FRAMEWORK

To construct inequivalent colorings of  $X$  fixed by  $K$ , we apply the following steps.

1. Determine the  $K$ -orbits of the elements of  $X$ .
2. Construct the partitions of  $X$  such that each element of the partition is a union of  $K$ -orbits, and use these partitions to construct colorings fixed by  $K$ .
3. For each  $K$  orbit, search for an element whose stabilizer is a subgroup of  $K$ . If such an element exists for each  $K$ -orbit, then the subgroup  $H$  of  $G$  that permutes the  $K$ -orbits is  $N_G K$ . Otherwise,  $H$  may be a larger subgroup of  $G$ , but always contains  $N_G K$ .
4. Compute the action of each element of  $H$  on the  $K$ -orbits.
5. From the action of  $H$  on the  $K$ -orbits of  $X$ , determine the equivalent colorings among the  $B_n$  colorings constructed in the second step.

### Conclusion and Recommendations

In this work, given a symmetric pattern and an arbitrarily chosen subgroup of its symmetry group, we developed a framework for constructing colorings of the pattern that are fixed by the said subgroup. We applied this framework on the sphalerite structure, and used the resulting colorings to perform ordered substitution. We observed the occurrence of some equivalences in the colorings using the normalizer of the chosen subgroup.

More research is necessary regarding equivalences of the resulting colorings. With the additional assumption in theorem 4, we deduced that the subgroup permuting the  $K$  orbits is precisely  $N_G K$ . It is interesting to study the opposite case where some  $K$ -orbits do not have elements with stabilizers contained in  $K$ .

The coloring framework may also be applied using other choices for the subgroup  $K$ , or using other structures aside from sphalerite. It may be a good idea to determine whether the resulting colorings correspond to known compounds, and if no such compounds exist, to establish whether the colorings may be realized into physical structures.

### Preliminaries

Let  $G$  be a group acting on a set  $X$ , and let  $x \in X$ .

- The  $G$ -orbit of  $x$ , denoted  $Gx$ , is the subset of  $X$  given by  $Gx = \{gx \mid g \in G\}$ .
- The stabilizer of  $x$  in  $G$ , denoted  $\text{Stab}_G x$ , is the subgroup of  $G$  given by  $\text{Stab}_G x = \{g \in G \mid gx = x\}$ .
- If  $K \leq G$ , the normalizer of  $K$  in  $G$ , denoted  $N_G K$ , is the subgroup of  $G$  given by  $N_G K = \{g \in G \mid gK = Kg\}$ .
- A coloring of  $X$  is a partition  $\mathcal{P} = \{P_1, P_2, \dots, P_n\}$  of  $X$ , where two elements of  $X$  are assigned the same color if and only if they belong to the same element of  $\mathcal{P}$ .
- [Roth, 1982] Two colorings  $\mathcal{P}_1$  and  $\mathcal{P}_2$  are called *equivalent* if the coloring  $\mathcal{P}_1$  may be transformed to the coloring  $\mathcal{P}_2$  by
  1. applying a symmetry element  $g$  of the symmetry group  $G$  to  $\mathcal{P}_1$ , or
  2. relabelling the colors in  $\mathcal{P}_1$  (i.e. changing the colors in a one-to-one fashion), or
  3. a combination of operations of type 1 and 2.
- An element  $g \in G$  is said to *fix the colors* if  $gP = P$  for each  $P \in \mathcal{P}$ .
- If  $H \leq G$ , we say  $\mathcal{P}$  is *fixed by  $H$*  or  $H$  *fixes  $\mathcal{P}$*  if every element  $h \in H$  fixes the colors in  $\mathcal{P}$ .
- (Bell numbers) The  $n$ th Bell number  $B_n$  is the number of partitions of a set of  $n$  elements.

### Sphalerite

Sphalerite ( $\text{ZnS}$ ) is a mineral whose crystalline structure resembles that of diamond. The symmetry group  $G$  of sphalerite is a space group of type  $F\bar{4}3m$ , generated by

1. the translations  $u$ ,  $v$ , and  $w$ ,
2. a four-fold roto-inversion  $f$  about the  $z$ -axis,
3. a three-fold rotation about the line connecting the origin and the opposite corner of the unit cell, and
4. the mirror reflection  $m$  along the plane  $y = x$  diagonal to the cube.

We choose  $K$  to be the subgroup generated by translations with a length of one unit along the  $x$  and  $y$ -axes, a translation twice the length along the  $z$ -axis, a translation from the origin to the center of the resulting box, the roto-inversion  $f$ , the half-turn  $h$  along the  $z$ -axis, and the reflection  $m$ . The subgroup  $K$  is a space group of type  $F\bar{4}3m$ .

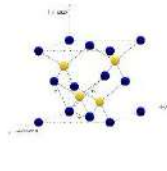


Fig. 1: A unit cell of sphalerite ( $\text{ZnS}$ ).

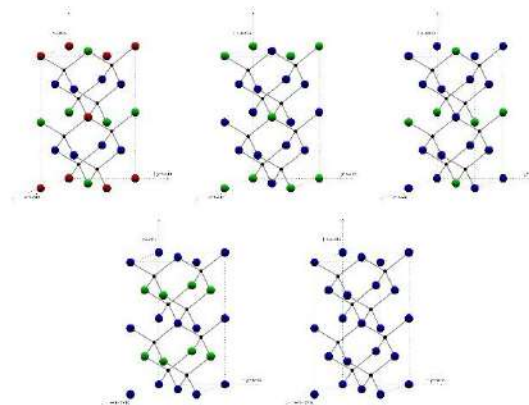


Fig. 2: The five colorings of the sphalerite structure fixed by the subgroup  $K$ . Observe that the second and third colorings are equivalent. The first coloring yields the structure of stannite ( $\text{Cu}_3\text{SnS}_4$ ), while the second gives cancrinite ( $\text{C}_4\text{H}_8\text{Al}_3\text{Si}_3\text{O}_{24}$ ).

### Acknowledgements

The presence would like to acknowledge the support of the organizers of the International School on Fundamental Crystallography: Seventh MathCryst School in Latin America, the Graduate School, PAFS, and the Office of International Education, and the University of the Philippines Diliman, in support of the Office of the Vice-Chancellor for Research and Development.

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Winning poster of O. Junio

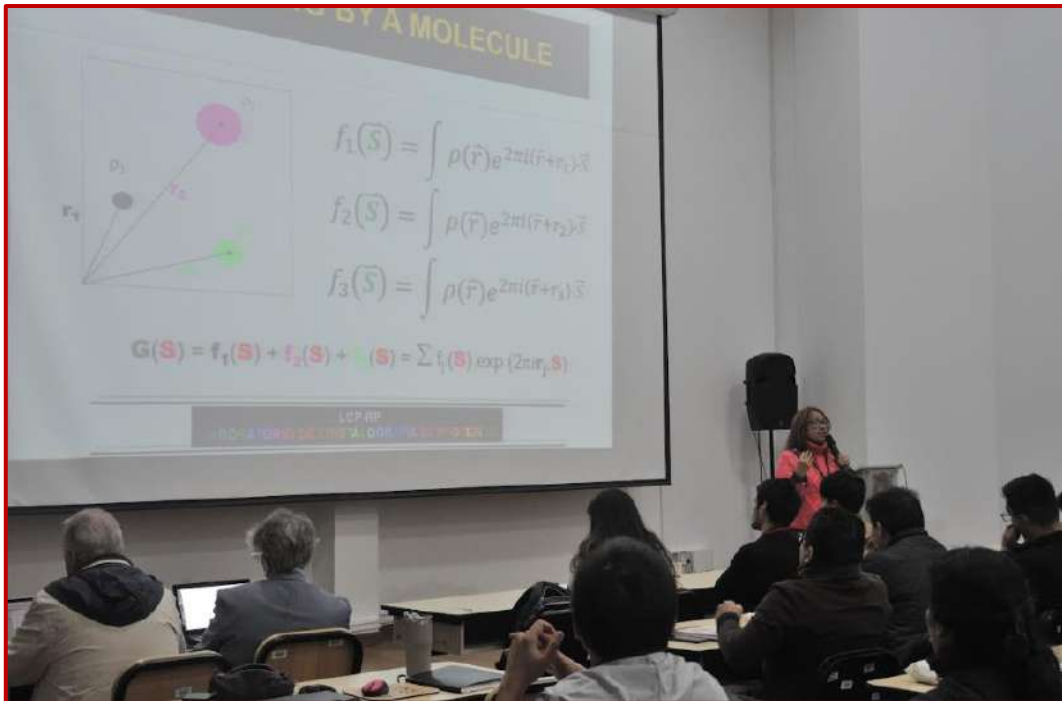
# PHOTOGRAPHS



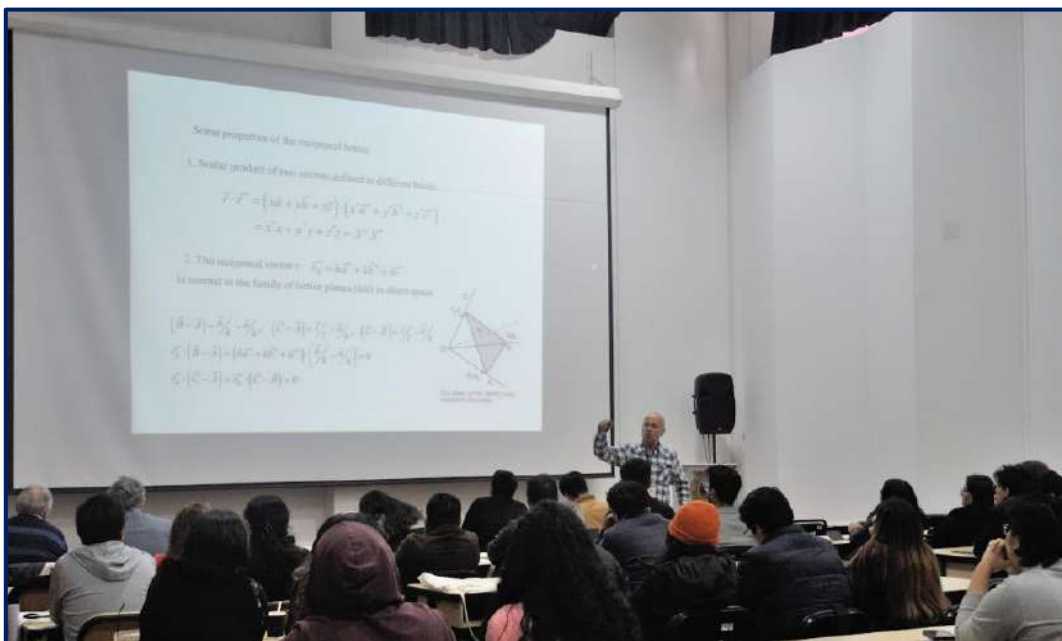
Inauguration of 7th MaThCryst School in Latin America. From left to right Dr. Arbelio Pentón, Dr. Leopoldo Suescun, Dr. Massimo Nespolo, Dr. Justiniano Quispe, Dra. Marisel Espinoza, Dr. José Niño, Dr. Ángel Bustamante, Mg. María Luisa Cerón, Dr. Moisés Arroyo, Dra. María Nonato y Dr. Carlos Landauro.





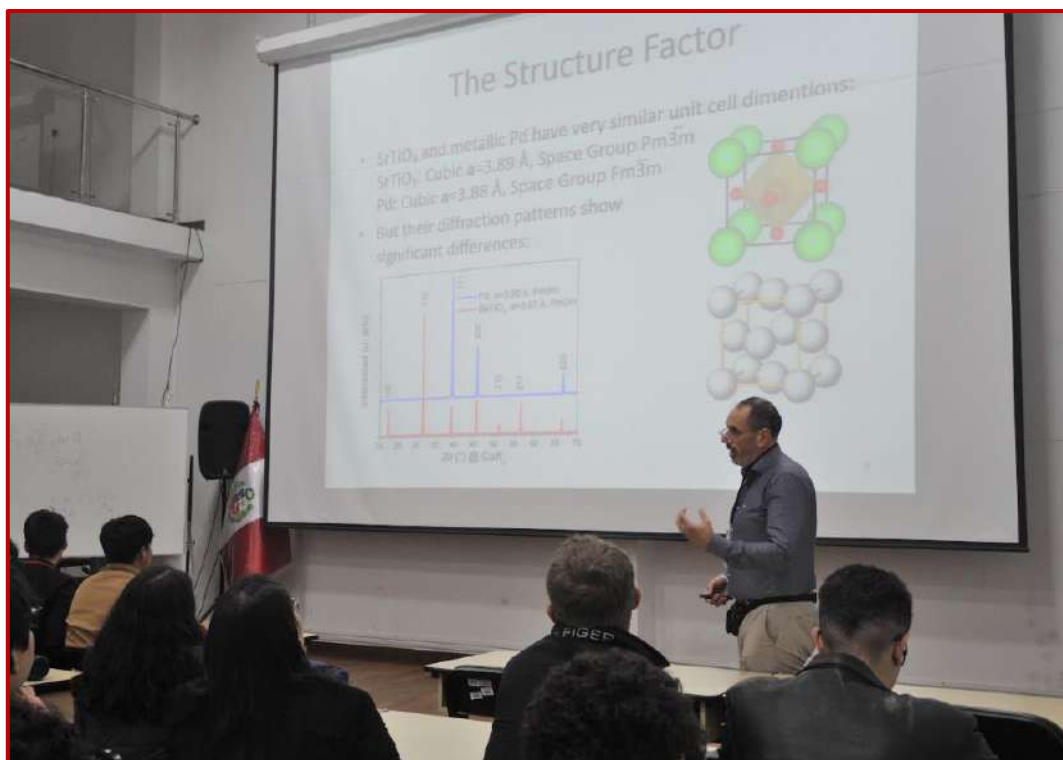


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**ABSTRACT BOOK OF INTERNATIONAL SCHOOL ON FUNDAMENTAL CRYSTALLOGRAPHY:  
SEVENTH MATHCRYST SCHOOL IN LATIN AMERICA - PERU 2024**



**August 12, 2024**



**August 16, 2024**

## VIDEOS



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SEVENTH MATHCRYST SCHOOL IN LATIN AMERICA - PERU 2024**

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