

Crystallography Online: Workshop on the use and applications of the structural and magnetic tools of the Bilbao Crystallographic Server

**University of the Basque Country (UPV/EHU)
2021, Leioa**

Lecturers (alphabetical order):

Mois I. Aroyo (MIA) (University of the Basque Country, UPV/EHU, Bilbao, Spain)

Gemma de la Flor (GF) (Karlsruhe Institute of Technology, Karlsruhe, Germany)

Josu Igartua (JI) (University of the Basque Country, UPV/EHU, Bilbao, Spain)

J. Manuel Perez-Mato (JMPPM) (University of the Basque Country, UPV/EHU, Bilbao, Spain)

Emre Tasci (ET) (Hacettepe University, Ankara, Turkey)

Irene Urcelay (IU) (University of the Basque Country, UPV/EHU, Bilbao, Spain)

Organizing Committee:

Jorge Lago (University of the Basque Country, UPV/EHU, Bilbao, Spain)

Irene Urcelay (University of the Basque Country, UPV/EHU, Bilbao, Spain)

Timetable:

Morning sessions (3.5 hours):

Lectures: 9:00 – 10:30 11:00 – 13:00

Afternoon sessions (3 hours):

Lectures: 14:30 – 16:30 17:00 – 18:00

Optional sessions (1 hour):

18:00 – 19:00

Coffee breaks: 10:30 – 11:00 16:30 – 17:00

Lunch: 13:00 – 14:30

SCIENTIFIC PROGRAM

Introductory day

morning session: Crystallographic symmetry: brief overview (MIA) (9:00-10:30; 11:00-13:00)

- Crystallographic point groups and their group-subgroup relations. Wyckoff positions of point groups.
- Brief introduction to magnetic symmetry and magnetic point groups.
- Space groups and their descriptions in *International Tables for Crystallography*, Vol. A. Transformations of the coordinate systems: change of origin and orientation. Conventional and non-conventional descriptions of space groups; ITA-settings.

BCS: hands-on session on the computer databases and access tools to crystallographic symmetry data for space groups (GENPOS, WYCKPOS, IDENTIFY GROUP)

afternoon session: Symmetry relations between space groups (MIA) (14:30-16:30; 17:00-18:00)

- Group-subgroup relations between space groups: Subgroups of space groups; maximal subgroups and Hermann theorem.
- Brief introduction to magnetic space groups.
- Domain-structure analysis in structural phase transitions.
- Relations of Wyckoff positions for a group-subgroup pair.
- Supergroups of space groups.

BCS: Hands-on session with the computer databases and computer tools in the study of group-subgroup relations of space groups (SUBGROUPGRAPH, SUBGROUPS, HERMANN, WYCKSPLIT, MINSUP, SUPERGROUPS).

18:00 - 19:00 (optional): Questions and discussion

Introductory day 2

morning session: Representations of crystallographic groups: basic concepts (MIA) (9:00-10:30; 11:00-13:00)

- Irreducible and reducible representations; characters of representations; subduced and induced representations; direct-product representations.
- Representations and character tables of crystallographic point groups.
- Mechanical and axial-vector representations.

BCS: Hands-on session with the computer tools of point-group representations (POINT, REPRESENTATIONS PG).

afternoon session: Representations of space groups (MIA) (14:30-16:30; 17:00-18:00)

- Representation of the translation group. Symmetry in reciprocal space: Brillouin zones and wave-vector symmetry types. Star of a representation. Little groups and small

representations. Full-group representations of space groups: representations of symmorphic and non-symmorphic groups.

- Subduced and direct-product representations of space groups.

BCS: Hands-on session with the computer tools of space-group representations (KVEC, Representations SG, REPRES, MECHANICAL REP).

18:00 - 19:00 (optional): Questions and discussion

1st day

morning and afternoon sessions: Crystal-structure tools of Bilbao Crystallographic Server (GF + ET) (9:00-10:30; 11:00-13:00) (14:30-16:30; 17:00-18:00)

BCS: Hands-on sessions with the computer crystal-structure tools

- Crystal-structure descriptions. Descriptions of crystal structures with respect to different ITA settings of the space groups (the program SETSTRU). Equivalent crystal structure descriptions (the programs EQUIVSTRU). Crystal-structure descriptions compatible with symmetry reduction (the program TRANSTRU). Comparison btw different structure descriptions (the program COMPSTRU).
- Crystal-structure relationships. Family trees (Baernighausen trees) of crystal structures: arystotype (basic) and hettotypes (derivative structures) (STRUCTURE RELATIONS).
- Possible symmetries of a distorted structure knowing only its non-distorted symmetry and the distorted lattice (SUBGROUPS) (Tutorial on the use of SUBGROUPS)
- Structural pseudosymmetry. Pseudosymmetry search for new ferroics. Application structural phase transitions (PSEUDO) (Tutorial on the use of PSEUDO).

18:00 - 19:00 (optional): Questions and discussion

2nd day

morning session: Crystal-structure tools: AMPLIMODES (JMPM + ET) (9:00-10:30; 11:00-13:00)

- Symmetry-mode description of distorted structures. Primary and secondary modes. Hierarchy of modes. Ferroelectric and ferroelastic phase transitions. Sequence of phase transitions (AMPLIMODES).

Tutorial on the use of AMPLIMODES

Tutorial on the visualization of the distortion modes obtained with AMPLIMODES

afternoon session: Crystal-structure tools (*cont.*) (JI) (14:30-15:30)

Practical case: Structural refinement with modes using FullProf and AMPLIMODES

Magnetic crystallography (JMPM) (15:30-16:30; 17:00-18:00)

- Magnetic point operations and magnetic point groups (MPOINT). Magnetic space groups. Types of magnetic space groups (MGENPOS, IDENTIFY MAGNETIC GROUP). BNS and OG settings in type IV magnetic space groups (BNS2OG). Wyckoff positions of magnetic space groups (MWYCKPOS). Extinction rules for magnetic space groups (MAGNEXT).

18:00 - 19:00 (optional): Questions and discussion

3rd day

morning session: Magnetic crystallography: modelling magnetic structures: (JMPM)
(9:00-10:30; 11:00-13:00)

- Possible maximal magnetic space groups for a given parent symmetry and a propagation vector and resulting magnetic structures (Tutorial on the use of MAXMAGN)
- Tutorial on the use of k-SUBGROUPSMAG plus MAGMODELIZE
- Representations analysis vs. magnetic symmetry description of magnetic structures. (MAGNETIC REP., Get_mirreps, kSUBGROUPSMAG with irrep filter) **(12:00-13:00)**

afternoon session: Magnetic crystallography (cont.) (JMPM) (14:30-16:30)

- Database of magnetic structures on the Bilbao Crystallographic Server. (MAGNDATA)
- Tensor properties of magnetic crystals (MTENSOR)

Magnetic crystallography (cont.) (IU)

Practical case: Refinement of a magnetic structure **(17:00 - 18:00)**

18:00 - 19:00 (optional): Questions and discussion