International Union of Crystallography
Commission on Mathematical and Theoretical Crystallography

Summer Schools on Mathematical Crystallography

Nancy, France, 21 June - 2 July 2010

International Union of Crystallography

European Crystallographic Association

Mineral and Inorganic Crystallography Special Interest Group

Association Française de Cristallographie

Crystallography Laboratory Nancy

Graduate School of Physics, Nancy-Metz

Graduate School of Molecular Chemistry and Physics, Nancy-Metz

On the occasion of the fifth anniversary of its foundation, the Commission on Mathematical and Theoretical Crystallography organizes two summer schools devoted to the **topology of crystal structures** and to the **irreducible representations of space groups**. The two schools will run one after the other, with pre-school optional days where the basic concepts necessary to attend the schools will be presented. Participants are welcome to present posters, which will remain on display during the whole period of the schools. Financial support for students and young scientists is available from IUCr, ECA and AFC funds.

Lecturers
Prof. Vladislav Blatov, Samara State University (Russia)
Prof. Davide Proserpio, Departement CSSI - University of Milan (Italy)
Prof. Mois Aroyo, Universidad del Pays Vasco (Spain)
Prof. Juan Manuel Perez-Mato, Universidad del Pays Vasco (Spain)
Prof. Boriana Mihailova, University of Hamburg (Germany)
Dr. Bernd Souvignier, Radboud University Nijmegen (The Netherlands)
Prof. Massimo Nespolo, Nancy-Université (France)

Local organizing committee
Prof. Massimo Nespolo, CRM2, Institut Jean Barriol, Nancy-Université
Ms Anne Clausse, CRM2, Institut Jean Barriol, Nancy-Université

The Organizers of the Nancy 2010 MaThCryst schools will 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 citizenship, religion, creed, political stance, ethnic origin, race, colour, language, age or sex, in accordance with the Statutes of the International Council for Science. At these schools no barriers will exist which would prevent the participation of bona fide scientists.

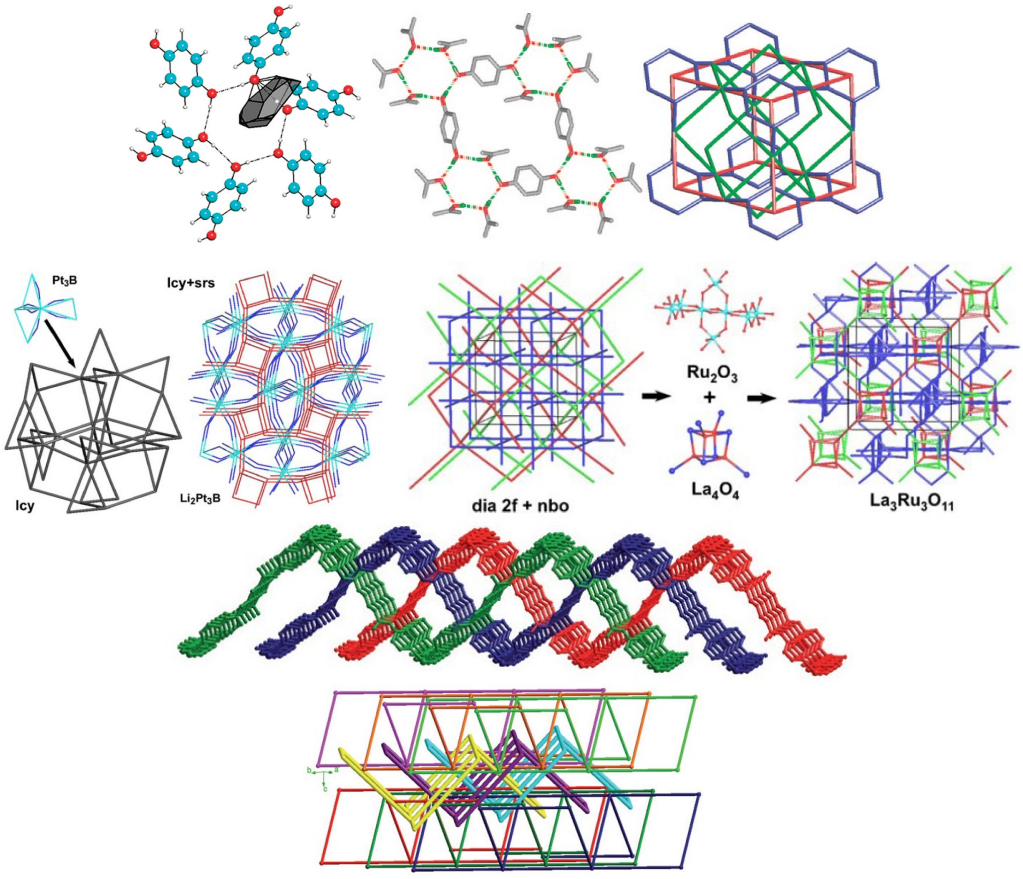
http://www.crystallography.fr/mathcryst/nancy2010.php

Topological Crystal Chemistry: Theory and Practice

The explosive growth in inorganic and organic materials chemistry has seen a great upsurge in the synthesis of crystalline materials with extended framework structures (zeolites, coordination polymers/coordination networks, Metal Organic Frameworks MOFs, supramolecular architectures formed by Hydrogen bonds and/or Halogen bonds etc.). There is a concomitant interest in simulating such materials and in designing new ones. However, it is a truism that before one can embark on systematic design of materials, one must know what the possibilities are. Indeed, in the last two decades there have been many parallel outcomes in the theoretical aspects of description and analysis of periodic structures (nets, tilings, surfaces, etc.), in the elaboration of databases, and in the development of software for analyzing and describing (illustrating) topological aspects of both real crystal structures and theoretical extended architectures. With these achievements, materials science and crystal chemistry comes up to a new level of their development that is characterized by deeper integration of mathematical methods, computer algorithms and programs into modeling and interpretation of periodic systems of chemical bonds in crystals.

The goal of this school is to give an introduction to this whole new area that we call ***Topological Crystal Chemistry***. There will be large time dedicated to hands-on session on the use of the novel and still not widespread computer methods/software/databases so the student at the end of the course should be able to analyze any kind of extended structure through the eye of the topology and describe it in term of nets, entanglements, catenation etc.

The target audience is young scientists (graduate students and postdoctoral associates) actively engaged in materials research, (experimental and/or theoretical) but also crystallographers who want to look at familiar structure types with a different eye. Some basic knowledge in chemistry and crystallography will be assumed which will provided during the pre-school day, for those needing a basic introduction.



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Irreducible representations of space groups

Group Theory is an indispensable mathematical tool in many branches of chemistry and physics. The school aims at giving the necessary background and practical skills for an efficient use of the group-theoretical methods in specific problems of solid-state physics, structural chemistry and material sciences. After a revision of the basic concepts of spatial symmetry and its description by crystallographic point and space groups according to International Tables of Crystallography, the principal results of the theory of group representations will be introduced with an emphasis on the practical aspects of the subject. Irreducible representations of crystallographic point and space groups and their derivation will be discussed in details. The abstract theory is limited to a reduced set of fundamental facts and statements. More attention is paid to different tools and techniques necessary for practical applications of the symmetry methods in solid-state problems as molecular dynamics, spectroscopy, electronic bands, phonon spectra, Landau theory of phase transitions.

The applications of group-theoretical methods to molecular vibrations including the concept of normal modes of vibrations will be discussed in details. The students will learn how, starting from symmetry requirements, to determine the spectral-transition selection rules with special attention to infrared and Raman spectra. The important role of representations of crystallographic groups in the classification, labeling and the analysis of the degeneracies of the lattice vibrations and electronic energy bands of crystalline solids will be reviewed. The applications related to phase transition studies will include the introduction of efficient techniques allowing the determination of the principle characteristics of a system undergoing a phase transition. For example, the determination of the order parameter from the knowledge of the initial and final phases, or the enumeration of all symmetry allowed phases that can result from a continuous phase transition. The symmetry-mode analysis of structural phase transitions results in the decomposition of the symmetry-breaking distortion, present in the distorted structure into contributions from different symmetry modes. The exposition of the general theory and methods will be illustrated with number of examples of typical phase transitions of different nature so that the participant can learn to apply the group-theoretical procedures in practice for the analysis of phase-transition mechanisms and in the search for new functional materials.

A tutorial and practical guide to the Bilbao Crystallographic server (www.cryst.ehu.es) forms an essential part of the course. The server provides an excellent on-line tool for the study of crystallographic symmetry and its applications. It gives access to databases with symmetry information on crystallographic groups, their group-subgroup relations and irreducible representations. The school aims at giving the necessary background and practical skills for an efficient use of the computer databases and programs on the Bilbao Crystallographic Server focused on solid-state physics and chemistry applications.

The participants of the school will benefit from the practical training in the application of advanced symmetry methods in solid state physics and crystal chemistry problems. The minimal mathematical prerequisites for the school widen the participation audience to students and researchers from chemistry, physics, geological sciences and engineering.

Program

The two schools will run one after the other, with a pre-school optional day where the basic concepts necessary to attend the schools will be presented. Participants to the pre-school day will be required doing some concrete exercises allowing them to get familiar with the bases that are assumed understood during the school. The weekend between the two schools will be devoted to presenting additional concepts that are pre-requisite to attend the second school. Participants familiar with these topics will be given the alternative of some optional excursions (not included in the registration fees).

Pre-school day

21 June: Introduction to crystal symmetry; space groups, Hermann-Mauguin symbols, exercises on the International Tables for Crystallography

Topological Crystal Chemistry: Theory and Practice

The first school will run on four days, from 22 to 25 June

THEORY

Periodic Structures and Crystal Chemistry... aka the Topological Approach to Crystal Chemistry
Graph, Nets & Tilings (Quotient Graphs & Natural Tilings)
Topological Analysis of Entanglement : interpenetration, polycatenation & more
Computer crystallochemical analysis: an overview
Applied computer crystallochemical analysis

P**RACTICE WITH PROGRAMS TOPOS, Systre, 3dt**

Module 1. Standard topological analysis and classification of nets in MOFs (Metal-Organic Frameworks), organic and inorganic crystals

Creating a database from CIF, SHELX or Systre formats
Computing adjacency matrix (complete set of interatomic bonds) for chemical compounds with different chemical bonding (valence, H bonding, specific interactions, intermetallic compounds)
Visualizing 0D, 1D, 2D and 3D structures
Standard simplified representations of MOFs or hydrogen-bonded organic crystals
Computing topological indices (coordination sequences, point, Schl?fli and vertex symbols)
Topological identification of nets. Working with TTD collection and Systre
Taxonomy of nets. Working with TTO collection

Module 2. Special topological methods of searching for building units in crystal structures

Special methods of simplification. Edge nets and ring nets. Analysis of synthons
Standard cluster representation of MOFs
Nanocluster representation of intermetallic compounds

Module 3. Analysis of entanglements in MOFs and molecular crystals

Visualization, topological analysis and classification of interpenetrating MOFs
Detection and description of other types of entanglement in MOFs: polycatenation, self-catenation and polythreading

Module 4. Analysis of microporous materials and fast-ion conductors with natural tilings

Computing natural tilings and their parameters. Visualizing tiles and tilings (TOPOS & 3dt). Simple and isohedral tilings. Constructing dual nets
Analysis of zeolites and other microporous materials, constructing migration paths in fast-ion conductors

Module 5. Crystal design and topological relations between crystal structures

Group-subgroup relations in periodic nets. Subnets and supernets
Maximum-symmetry embedding of the periodic net, working with the Systre program
Mappings between space-group symmetry and topology of the periodic net
Searching for topological relations between nets and working with net relation graph
Applications of net relations to crystal design, reconstructive phase transitions, taxonomy of crystal structures

Participants are invited to bring their own data/structures to be analyzed as well as personal computers to install the software.

Weekend intermission

26-27 June: preparation to the second school

A. **Basic facts on crystallographic groups**

A.1. Point groups. Elements of point symmetry. Groups, subgroups and theorem of Lagrange. Generators. Classes of conjugation. Abelian groups and cyclic groups. Crystallographic point groups and abstract groups. Generation of point groups by composition series. Classification of crystallographic point groups.

A.2. Crystallographic symmetry operations and their presentation by matrices. Space groups. Translation groups and coset decompositions of space groups. Symmorphic and non-symmorphic space groups. Generation of space groups by composition series.

A.3. Group-subgroup relations of point and space groups.

Irreducible representations of space groups

The second school will run on five days, from **28 June** to **2 July**

B. **Representations of crystallographic groups** (3 days)

B.1. General remarks on representations. Representations of discrete groups. Equivalence of representations. Unitary representations. Invariant subspaces and reducibility. Theorem of orthogonality. Characters of representations and character tables.

B.2. Representations of point groups. Representations of Abelian groups: cyclic groups and direct products of cyclic groups. Character tables of representations of point groups. Online databases for point-group representations.

B.3. Induction procedure for the derivation of the representations of crystallographic groups. Subduced and induced representations. Conjugate representations and orbits. Little groups, allowed representations and induction theorem. Induction procedure for indices 2 and 3. Representations of some point groups by the induction procedure.

B.4. Representations of space groups Representation of the translation group. Star of a representation. Little groups and small representations. Representations of symmorphic and non-symmorphic groups. Online tools for the derivation of space-group representations.

C. **Applications of representations theory in solid-state physics and chemistry** (2 days)

C.1. Vibrations in molecules and solids

C.1.i. Molecular dynamics. Small oscillations and normal modes. Zero modes and vibrational modes. Mechanical and vibrational representations. Dynamical matrix in symmetry adapted coordinates. Degeneracy.

C.1.ii. Electronic energy bands and phonon spectra. Assignment of small representations. Compatibility relations. Symmetry-adapted bases. Partial diagonalization of the dynamical matrix. Anticrossing.

C.1.iii. Direct products of irreducible representations and selection rules - general formulation. Selection rules in molecular spectroscopy: rotational and vibrational absorption, infrared and Raman effect. Direct products of space-group representations and selection rules. Online tools for infrared and Raman selection rules.

C.1. Structural phase transitions

C.2.i. Representation theory tools in the analysis of phase transitions. Primary and secondary order parameters; couplings and faintness index. Order parameter direction and isotropy subgroups. Group-theoretical formulation of the necessary conditions for second-order phase transitions.

C.2.ii. Symmetry-mode analysis of structural phase transitions. Hierarchy of modes. Symmetry-modes applications in structure refinement. Online tools for symmetry-mode analysis.

Poster presentations

Participants are welcome to present posters, which will remain on display during the whole period of the schools. Abstracts for the posters have to fit one page A4 size and should follow the templates available from the schools website as OpenOffice writer, Rich-Text Format and Microsoft Word files. Abstracts should be submitted by email ; they will be collected in a PDF file and made available for download from this website after the schools.

Language

The official language of the schools is English. No simultaneous interpretation will be provided.

Venue

The summer schools will be held at the Amphitheatre No. 8 of the Faculty of Sciences of the Université Henri Poincaré Nancy I (GPS coordinates: Latitude 48.6653088, Longitude 6.1589755). The Faculty campus is located at Vandoeuvre-les-Nancy, in the immediate suburb of Nancy, and can be reached from Nancy railway station in about 15-20 minutes. Details available from the schools website

Accommodation

Close to the Faculty campus several accommodation facilities are available, including: student dormitories.

- *La Maison des Chercheurs*, in front of the Campus, offers studios (20 m2) and suites (30 m2) equipped with bathroom, small fridge, electric cooking plates and kitchen commodities.
- *Le Château de Rémicourt* is a youth hostel with 60 rooms at budget fare.
- *The Cottage hotel* is a two star hotel at the Brabois plateau, close to the terminal station of the tram, not far from the campus.
- *The Akena Hotel* is suitable for those who prefer to stay close to Nancy railway station.
- Rooms in several *student dormitories* around the campus can be booked via the organisers but the level of comfort and the services offered are minimal.
- Other hotels can be booked via the *Nancy tourist office*.

Warning: On June 21st a "music festival" is held in all towns in France: the night between the 21st and the 22nd the city centre will be animated and quite noisy until 2 a.m.

Visa

Citizens of the European Union, of the European Economic Space, and of Switzerland do not need a visa to enter France. Participants who need an invitation letter to obtain a visa should send a request to: Mme Anne Clausse, CRM2 UMR-CNRS 7036, Institut Jean Barriol, Nancy Université, BP 70239, F54506 Vandoeuvre-lès-Nancy cedex, France, with a letter of motivation, their curriculum vitae, a list of publications or (for students) a recommendation letter signed by the supervisor, a copy of the passport pages with personal data and photo. ***Incomplete requests or requests by people whose curriculum and field are unrelated to the topics of the school will not be treated.***

Financial support

Limited financial support will be available for students and young scientists. Applicants for financial support must be registered in the *World Directory of Crystallographers*: registration is free of charge and takes only a few minutes. Grants from funds by the European Crystallographic Association (ECA) will be assigned with priority to *Individual Members of the ECA*. The *French Crystallographic Association* offers 4 grants of 150 € each to *French students or post-doctoral fellows* (age limit 35 years old, not holding a permanent position) provided that the applicant or the supervisor is member of the Association. Applicants should contact the Association directly.

Contact

Inquiries about the scientific program of the schools should be sent to Mathcryst.Commission@crm2.uhp-nancy.fr. For inquiries about lodging and logistic please contact Anne.Clausse@crm2.uhp-nancy.fr.