# Online Teaching Aids for Crystallography

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## Outline

- Introduction. The challenges of teaching crystallography at University level.
- What teaching aids can we find currently on the web ?
- Crystallographic applets on the web.
- Components of a basic course in crystallography.
- The Lausanne eCrystallography course.
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## The challenges of teaching crystallography at University level

- As an interdisciplinary branch, crystallography is taught to a broad spectrum of students in
  - Physics
  - Chemistry
  - Material science
  - Earth science
  - Life science
- Each class of student is interested in some specific aspects of crystallography, for example
  - direct methods are important for chemists but of lesser interest for physicists
  - Material scientists are mainly concerned with powder diffraction whereas life science students are interested in single crystal diffraction and a limited amount of space groups...





## Knowing that the students

- are very familiar with the web environment
- use Internet as a primary source of information
- prefer to download information freely available from the web instead of buying expensive textbooks

## How can we take advantage of the net to prepare useful teaching resources?

## Possible answers

- Use or develop applets (small platform independent applications directly run from a browser) illustrating or simulating specific aspects of crystallographic concepts
- Combine them with open source database (e.g. BCS, LCS,...)
- Both teacher and students can use the applets at their convenience

## What teaching aids can we find currently on the web ?

Many resources dedicated to crystallography exists on the web

- Monographies (*e.g.* IUCr teaching pamphlets)
- Videos (*e.g.* YouTube Broadcast Yourself™ )
- Online calculations from remote servers (*e.g.* Discus server)
- Applets
- Databases including retrieval tools (BCS, LCS, ICSD,
- online toolboxes for better interactivity
- Etc.

All these possibilities can be demonstrated in real time in order to illustrate specific items in a course.



## Crystallographic applets on the web

Owing to the ever increasing power of PCs, applets can do very elaborate type of calculations like

- Diffraction simulation, Fast Fourier transform
- Structure representations, Fast 3-d rotations of objects (crystals, large molecules,...)
- Other simulations

Since more than a decade, many crystallographers have developed applet directly available on the net

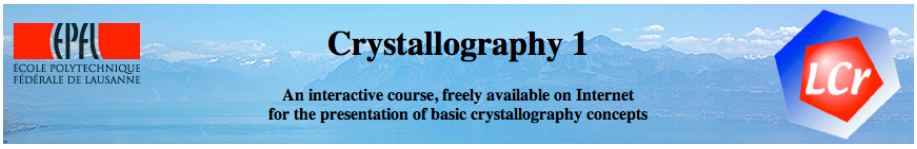
- Steffen Weber (http://jcrystal.com/steffenweber/java.html)
- Kevin Cowtan (http://www.ysbl.york.ac.uk/~cowtan/)
- Nicolas Schoeni & Gervais Chapuis (http://escher.epfl.ch)
- And many more

# The basic ingredients of an introductory course in crystallography include

- **Symmetry.**
  - Point and space group symmetries
- **Diffraction**
  - Fourier transform
  - Diffraction methods
  - Phase identification methods
  - Structure solution methods
- **Examples** of crystal structures
  - monoatomic, binary or ternary compounds
  - Compact sphere packings and derivatives
  - Tetrahedral and octahedral interstices








The eCrystallography course is based on a series of applets each one illustrating some specific concepts on

Symmetry
- Escher Web Sketch 2
- Initiation to the discovery of symmetry
- Stereographic projection

Diffraction
- Diffraction and Fourier Transform
- Reciprocal lattice generator
- Ewald sphere animation
- diffractOgram
- Fourier synthesis
- reciprOgraph

Structure solutions
- Charge flipping

Structure handling
- crystalOgraph
- Powder diffraction files
- cellConverter

## The Lausanne eCrystallography course (2)

The eCrystallography course is more than a series of applets

- It is a complete course with interactive exercises
  - There are some 50 exercises
  - Other complementary applets available on the web are also accessed
- Each concept is introduced successively and can be immediately tested
  - Each individual can learn at his own pace
  - A forum on the web, specific to the course, has been set up and can be used for exchange of information between teachers and students or between students
- It can be used by teachers during his lecture, either in parts or for the the complete course.



## Exercise 1

Let us derive the general and special positions of the planar group *p*6mm.

Hint for the solution

1. Use the applet Escher web sketch ( http://escher.epfl.ch/escher/). Select the corresponding planar group and the  tool.
2. Derive the general positions in an hexagonal unit cell, how many?
3. Find all the special positions with EWS
4. Check your results with the BCS ( http://www.cryst.ehu.es/cryst/get_wp.html)

## Exercise 2

Show that the point group operation $\bar{4}$ does not contain the inversion. It can however be obtained by combining an inversion and a 90° rotation along the $\bar{4}$ axis.

### Hint for the solution

1. Use the Symmetry Discovery applet ( http://escher.epfl.ch/symmetry/). Select an object with the $\bar{4}$ symmetry operation.
2. Use the applet tools to transform the object



## Exercise 3

Given a crystal class, explore the effect of a form by modifying a point on the stereographic projection

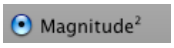
### Hint for the solution

1. Use the Steffen Weber applet ( http://jcrystal.com/steffenweber/JAVA/jpoly/jpoly.html) and select one of the possible crystal class
2. Use the mouse to place and move a point on the stereographic projection and see the effect on the right panel.
3. The form can be moved with the mouse in the right panel.

## Exercise 4

Generate the Patterson function of a simple structure and study the effect of the atomic number of the atoms

### Hint for the solution

1. Use the Fourier transform applet (http://escher.epfl.ch/fft/). On the left panel, create a simple structure with three or four atoms.
2. The FFT button generate the FT in the right panel.
3. The corresponding Patterson function, can be obtained by selecting the 

and then the 

buttons.
4. Test the effect of atomic weights on the Patterson function.



## Exercise 5

Given a unit cell, generate the corresponding reciprocal lattice vectors

### Hint for the solution

1. Use the Reciprocal lattice calculator applet ( http://escher.epfl.ch/rlattice/). Select one of the periodic patterns and follow the instructions.
2. You can always select between various modes of displays, *i.e.* pattern, lattice or reciprocal lattice

## Exercise 6

Use the Ewald sphere construction to simulate Laue diagram in reflexion and a Debye-Scherrer diffractogram

Hint for the solution

1. Use the DiffractOgram applet ( http://escher.epfl.ch/diffractOgram/). On the “Screen” panel, select a negative crystal-film distance (*e.g.* 4 cm). Hit the Laue button in the “Animation” panel. You can increase the number of reflexions by hitting “more” in the “Lattice” panel.
2. A classical Debye-Scherrer film can be obtained by selecting the ”Cylindric” screen, with a wavelength of at least 1.50 Å. Hit then the “Debye-Scherrer” button.



## Exercise 7

Study the effect of individual terms in a Fourier synthesis representing the electron density.

Hint for the solution

1. Use Kevin Cowtan’s applet ( http://www.ysbl.york.ac.uk/~cowtan/sfapplet/bigframe_miller.html). In the upper right panel, select first the *hk* indices.
2. In the lower left panel, select the corresponding phase and amplitude of the structure factor. Observe the effect of the phase and amplitude terms on the lower right panel.
3. Hit the Set SF button to include the term in the Fourier summation. Continue with additional terms

## Exercise 8

Derive the systematic absences of the NaCl (or any other) structure.

### Hint for the solution

1. Use the ReciprOgraph applet ( http://escher.epfl.ch/reciprOgraph/). In the “Files” panel, select “ICSD” and then the “NaCl” structure. Hit the “Import selected” button.
2. The systematic absences can be deduced by inspection of the reciprocal lattice weighted by the intensities. Each layer can be easily inspected with the cursor.
3. The ICSD button allows you to search and analyse other structures available in the database.



## Exercise 9

Study the role of the single parameter δ in the structure solution method by charge flipping

### Hint for the solution

1. In the above left panel of the charge flipping applet ( http://escher.epfl.ch/flip/) use the drawing tools to create a structure from which the moduli of the structure factor will be calculated. Hit the “Loop” button to solve the structure in automatic mode by CF.
2. Hit the “Reset” button and increase the value of the “parameters” panel and study its effect on the structure solution.

## Exercise 10

Find the range of the shortest S-S bonds in the structure of S (Warren, 1935)

Hint for the solution

1. The applet (http://escher.epfl.ch/crystalOgraph/) can be used to represent the structure. Hit 

and look for the 1935 entry of Sulfur. Import the structure.
2. Hit “More” in the “Bonds” panel. Repeat this action until all the shortest bonds are identified.
3. Compare the space group operations (hit “CIF file”) with the corresponding SG in the BCS database. Try to locate the inversion center of the space group.



## Exercise 11

Find the new atomic coordinates of NiAs in an orthorhombic C-centered cell with additional origin shift

Hint for the solution

1. Use the applet (http://escher.epfl.ch/cellConverter/) and select the NiAs structure from “File→Get from ICSD”. Insert the proper matrix transformation and origin shift to obtain the new atomic coordinates in space group *P*1.
2. Compare the CIF files before and after the transformation

## Exercise 12

Simulate the powder diagram of a structure extracted from ICSD

### Hint for the solution

1. Select (http://escher.epfl.ch/reciprOgraph/) and look for an ICSD structure. Import the selected structure and hit 




## Conclusions

### After some years of practice at EPFL

- Students appreciate the visualisation aspects of the course
  - To understand the meaning of point and space group symmetry
  - For the representation and analysis of the structures
  - For a better understanding of diffraction phenomena
- In order to get familiar with the eCrystallography course environment students need some practical help before starting
- The course should be completed by further readings in classical textbooks

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# Questions