TEACHING AND EDUCATION IN CRYSTALLOGRAPHY

Contributions intended for this section should be submitted to the Teaching and Education Editor, whose address appears on the inside front cover of the journal. They may describe any aspect of the teaching of crystallography and may take the form of short communications, teaching notes or full research publications.

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Crystallographic CourseWare

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Abstract

Crystallographic CourseWare is a set of computer animations and interactive exercises designed to assist undergraduate and introductory graduate students in their learning of crystallography. Topics discussed include crystal growth, plane- and space-group symmetry elements, unit cells and asymmetric units, reciprocal space, precession photographs, and an introduction to reading the *International Tables for Crystallography*.

1. Introduction

Do you teach crystallography? Who are your students? What do they need to learn? What do they need to be able to do with that knowledge? How much time do you have to teach them? What mode of instruction do you want to employ? What instructional materials are available to help them learn?

My students are undergraduate and master's level chemistry majors. Few will ever solve structures by themselves, but all will read the chemical literature and will benefit from an understanding of crystallographic results. Many will become synthetic chemists who are likely to collaborate with crystallographers. Owing to constraints in the undergraduate curriculum, crystallography usually can be offered as a special topic at best. I normally teach crystallography as a half-course seminar every two or three years or offer it as an independent study course. This severely restricts the time available for instruction and requires a high degree of selectivity as to topics discussed and depth of presentation. However, the small class size and seminar designation allow me to explore 'student-centered learning' as a major pedagogical goal. The goal of 'student-centered learning' is to change the role of teacher from lecturer to coach and the role of student from passive recipient of information to active participation in the learning process (Moore, 1989; Lagowski, 1998). Standard textbooks are well suited to prepare professional crystallographers. However, the extensive mathematical treatment in the text and the lack of appropriate practice exercises makes them less suitable for general chemists. These answers to the above questions have led me to develop two videotapes and a set of computer demonstrations and exercises called *Crystallographic CourseWare*.

The primary focus in *Crystallographic CourseWare* is on symmetry and derived results. The discussion of diffraction theory and experimental techniques is limited to a practical understanding of the vocabulary. The computer programs are not intended to replace a traditional textbook entirely, but rather to provide an alternative learning-style resource for specific topics. They exploit the capacity of computer animation and interactivity to engage the student actively in learning selected topics. The programs can also be used for homework assignments for traditional courses or as a major component of an independent study course.

2. Course notes

The following describes the materials and how they have been employed.

2.1. *Introductory overview*

A videotape (Kastner, 1992) presents the general process of structural solution and helps to provide a general framework for the course. The discussion includes selection of a crystal, precession photographs and data collection on a four-circle system, electron density maps and difference maps, and final computer models.

2.2. *Crystal growth*

The unit on crystal growth, while clearly applicable to a crystallography course, can also be used with student 'consumers' of crystallography. Helping students to grow quality crystals is often an iterative process. Typically, a student working in a colleague's synthetic laboratory will walk in with a reaction vessel and say 'See these crystals? Can we get a structure?' Following a brief explanation of the desirability for quality single crystals, students can be directed to 'crystal growth' in *Crystallographic CourseWare*. This program presents animations and text describing several methods for growing crystals. Fig. 1 presents selected frames from the animation on vapor diffusion. Color coding (somewhat obscured in this black-and-white rendition) is used to help demonstrate the concept. The idea of a poor (yellow) solvent diffusing into a good (blue) solvent to make a mixed (green) solvent system seems to be easily understood by students. After working through 'crystal growth', students clearly recognize the need to know the solubility characteristics of the compounds and can identify which of the techniques discussed seem most appropriate for their compound. Subsequent conversations based on the observations of their attempts help them 'tweak' the system and usually lead to reasonable crystals.

2.3. *Symmetry elements*

The *CourseWare* unit introducing symmetry elements exploits multimedia and non-linear options available in computer presentations. As an example, the screen used for the twofold screw is shown in Fig. 2. Four components of symmetry for the element are presented. A brief definition is given in the upper right-hand corner. A graphic displays the images of hands along with the standard single-barbed arrow symbol of the twofold screw. Shading is used on the upper hand image to indicate that it is further down on '*c*' than the lower hand images. Clicking on the icon of the movie projector brings up a short animation; see Fig. 3. *International Tables for Crystallograhy* (Hahn, 1983) symbols of open circles are shown in the same orientation as the hands. Clicking on the 'more information' button brings up a description of the algebraic representations for the general positions (x, y, z; $0.5 + x$, $-y$, $-z$). Students can choose to look at all four components for one element by systematically moving deeper into the page. Alternatively, students can be encouraged to make three passes through the unit. On a first pass they would look at definitions and hand images for all of the elements. Next they would compare the hand images with the circle representations. Lastly they would look at the coordinates.

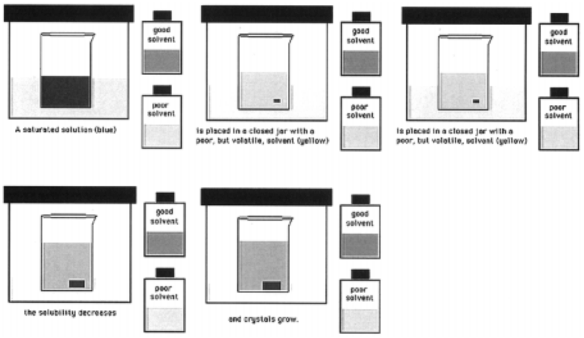
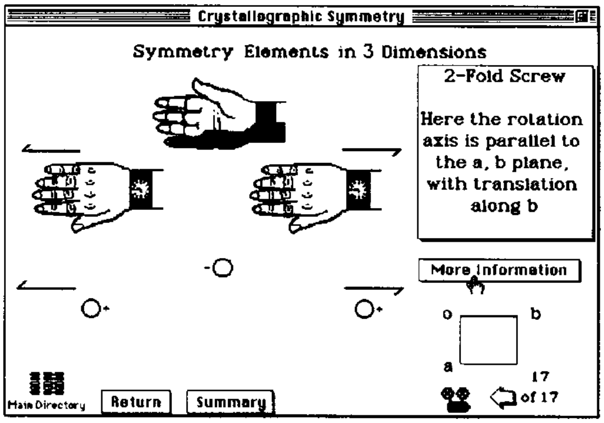


Fig. 1. Selected frames from one animation on crystal growth.

2.4. *Unit cells, asymmetric units and exercises in plane-group symmetry*

Once students can identify symmetry and repeating units in two dimensions it is easier for them to envision a three-dimensional system. The *CourseWare* program on unit cells and asymmetric units uses animation to demonstrate (1) locating all of the symmetry in two-dimensional pattern, (2) connecting equivalent elements to outline the unit cell and (3) using the symmetry within the cell to divide it into asymmetric units. Students are then presented with a simple motif in each of the 17 plane groups. For example, in Fig. 4, plane group *p*2*mg* is shown partially solved (bottom). Two vertical glides, two


Crystallographic Symmetry

Symmetry Elements in 3 Dimensions

2-Fold Screw

Here the rotation axis is parallel to the a, b plane, with translation along b

Fig. 2. Selected screen from the introduction to symmetry elements.

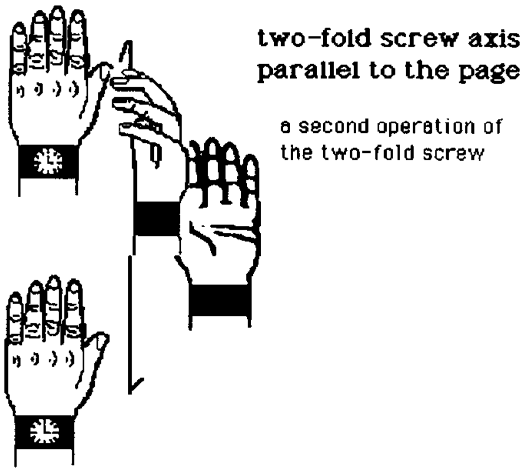


Fig. 3. One frame of the animation for the twofold screw.

horizontal mirrors and nine of the twofold rotations have been positioned in the example shown. The symbols are positioned by clicking first on a symbol button in the tool box (top right) and then clicking at the appropriate locations on the pattern. Students can check their work with the on-line answer (top left). Clicking on the movie projector icon brings up an animation showing the details of the solution. Additional units discussing special positions and three-dimensional patterns are in production.

2.5. *Exercises in reading International Tables for Crystallography, Volume A*

The introductory material given in the *International Tables for Crystallography* (Hahn, 1983) and by Hahn & Wondratschek (1994) provides a very detailed and mathematically precise background for space-group symmetry. Although some students have the mathematical aptitude to understand this presentation, many chemistry students who desire to understand space-group symmetries find the mathematical presentation difficult. The exercises presented in *Crystallographic CourseWare* provide a visual, tactile approach to understanding the *International Tables for Crystallography*. Fig. 5 presents selected frames from the animated answer to the plane group *c2mm* exercise. This animation is designed to help the student understand the transition from two-dimensional patterns of the type shown in Fig. 4 to the conventional symbols for space groups, as shown in Fig. 6.

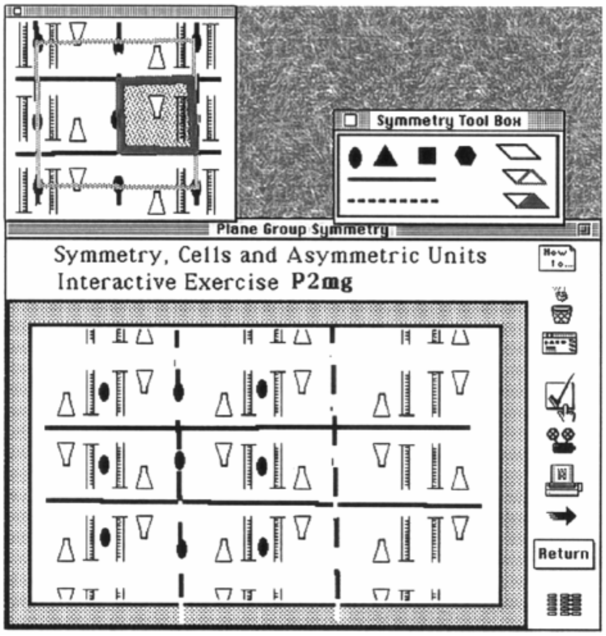


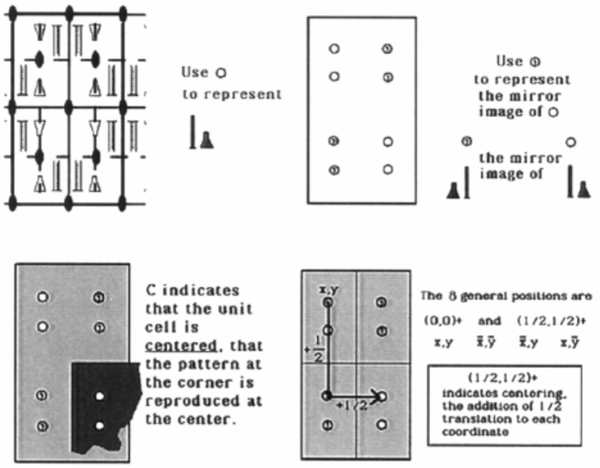
Fig. 4. A template for exercises in plane-group symmetry (bottom), the toolbox (top right) and the answer (top left).

Fig. 6 shows an example of a practice exercise in reading the diagrams for typical space groups in the *International Tables for Crystallography*, Volume A. Fig. 6(*a*) shows a symmetry diagram on the left (the question) and a template for the general position diagram (the answer) on the right. By clicking on the symbols in the box at the top, the student can construct the general position diagram. Only two of the general position symbols have been positioned on the right side. In Fig. 6(*b*) the on-line answer is shown on the left. Many similar exercises are provided. Given one of (*a*) coordinates, (*b*) general positions diagram, or (*c*) symmetry diagram, students are asked to construct one of the others. Answers are on-line for some of the exercises. Answers to others are available in the *Brief Teaching Edition of Volume A* (Hahn, 1993). This is to encourage students to use and become more familiar with that resource. Some exercises can be found only in Volume A (Hahn, 1993) and can be used as quizzes, assuming Volume A is not available to the students.

2.6. *Reciprocal space*

The physics of diffraction is important to understanding the experimental design and theory of crystallography. Neder & Proffen (1996) describe programs designed to teach diffraction. At a minimum, students should understand that the reflections in the diffraction pattern are the data. Precession photographs provide the most direct, visual experimental data and are arguably the easiest to interpret. From precession photographs one can measure the cell constants, determine the space group based on systematic absences, and can observe that reflections have differing intensities.

Few laboratories have maintained precession cameras and even those that have may debate the value of spending the time required to do the orientation and



C indicates that the unit cell is centered, that the pattern at the corner is reproduced at the center.

The 8 general positions are

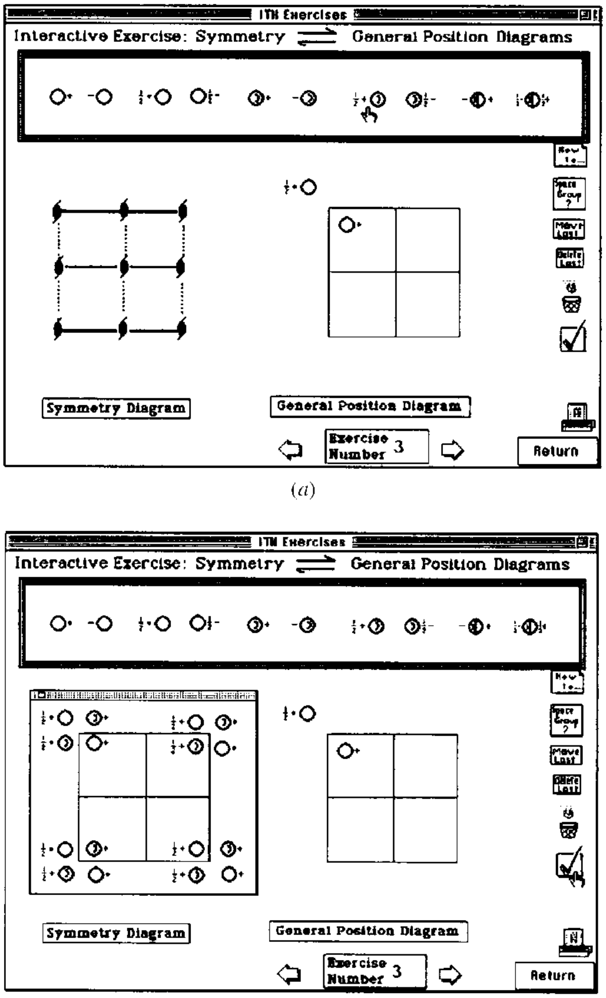
(1/2,1/2)+ indicates centering, the addition of 1/2 translation to each coordinate

Fig. 5. Selected frames from an animation showing the relationship between a simple repeating motif and the standard symbols used in *International Tables for Crystallography*.

centering of crystals. A videotape (Kastner, 1989) designed to teach students how to take photographs is useful to students even if they do not get the hands-on experience of using a camera. The program also demonstrates how cell constants are measured from the photographs and discusses systematic absences noted for the sample used. An inexpensive exercise which can be used to help demonstrate cell constants and systematic absences is an optical transform kit (Lisensky *et al.*, 1994). This exercise is also far less time-consuming than precession-camera work.

To help with an understanding of the relationship between the real crystal lattice and the precession photograph, one unit of *Crystallographic CourseWare* shows a step-by-step construction of reciprocal space taken from a discussion presented by Stout & Jensen (1989). One frame from this discussion is shown in Fig. 7. In a standard lecture the instructor might construct a similar diagram on a black board or with overheads. However, with the computer presentation the student can look at any step for as long as desired and, if the instructor is available, ask questions on a one-on-one basis while other students progress at their own pace. This simple presentation provides at least some foundation for the discussion of the diffraction pattern as observed in precession photographs.

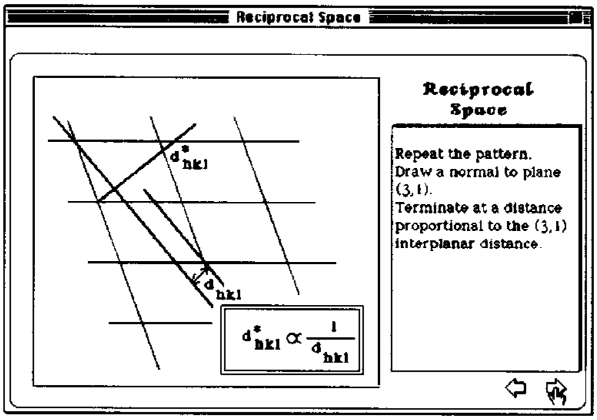
The unit on precession photographs then describes how to index the photographs and allows users to verify their understanding by clicking on particular reflections with appropriate feedback given. Simulations of precession photographs are used to compare zero-level with upper-level photographs and locate systematic absences. One example rotates an octant of reflections to show the three-dimensional array. Fig. 8 shows



(*a*)

(*b*)

Fig. 6. Templates for exercises in reading the *International Tables for Crystallography*.



Repeat the pattern.
Draw a normal to plane (3,1).
Terminate at a distance proportional to the (3,1) interplanar distance.

Fig. 7. One frame from the reciprocal-space unit.

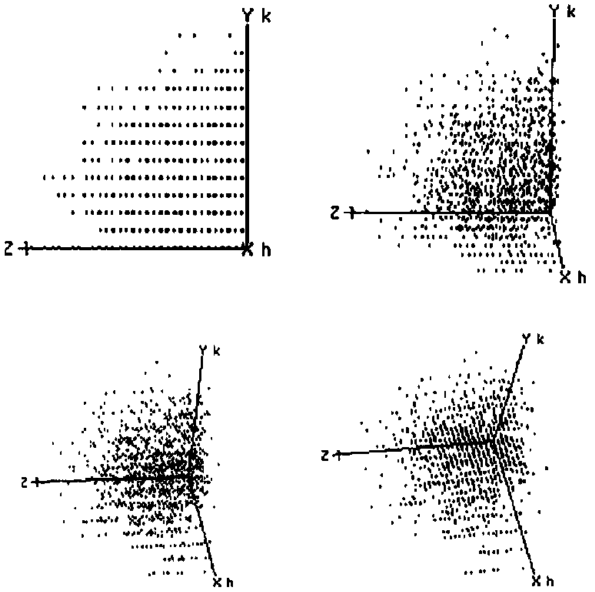
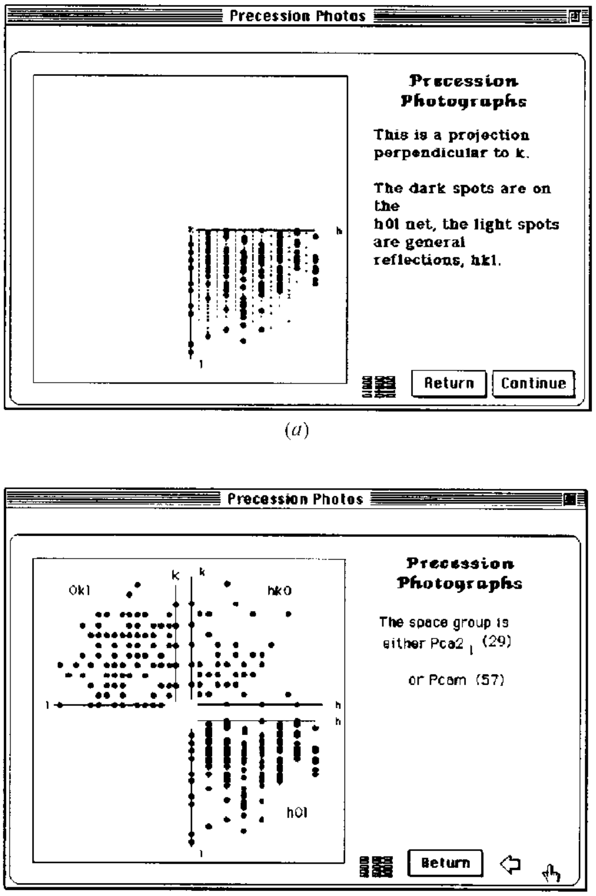


Fig. 8. Selected frames from the rotation of an octant of reflection data.

selected frames from this rotation. The relationship between this array and the zero-level photographs is discussed. For example, Fig. 9(*a*) shows one face, the zero level, of this octant in bold with upper-level reflections as lighter or background dots. The systematic absences are discussed in terms of the symmetry indicated by their absence. Fig. 9(*b*) shows the concluding frame of this discussion, with the assignment of possible space groups indicated.



Precession Photographs

This is a projection perpendicular to k.

The dark spots are on the h0l net, the light spots are general reflections, hkl.

(*a*)

Precession Photographs

The space group is either $Pca2_1$ (29) or Pcam (57)

(*b*)

Fig. 9. Selected frames from the precession-photographs unit.

3. Availability of teaching materials

Windows and Macintosh versions of *Crystallographic CourseWare* have been submitted to the *Journal of Chemical Education: Software*. Information on the current status is available from the web site: www.facstaff.bucknell.edu/kastner.

4. Conclusions

The computer programs described can be an effective tool to assist students in learning crystallography. The programs can be used as the major component of a student-centered learning course, as homework exercises for a traditional course, or for independent study. The programs combine animation and interactive exercises to provide an alternative to the standard mathematical treatment of symmetry.

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