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Crystallography Collection

Abstract of Special Issue 26 on CD-ROM

In This Issue

Crystallography Collection, Special Issue 26, consists of two programs for Mac OS and Windows: Point Group I, II, and III and Crystallographic CourseWare.

Point Group I, II, and III is a series of programs designed to teach point-group symmetry. The first two units are appropriate when symmetry elements are introduced. The third helps students assign a point group to a structure.

Crystallographic CourseWare teaches fundamental crystallographic concepts at an upper-division undergraduate level, or for graduate students.

Price and Ordering

An order form is inserted in this issue that provides prices and other ordering information. If this card is not available or if you need additional information, contact *JCE Software*, University of Wisconsin–Madison, 1101 University Avenue, Madison, WI 53706-1396; phone; 608/262-5153 or 800/991-5534; fax: 608/265-8094; email: *jcesoft@chem.wisc.edu*.

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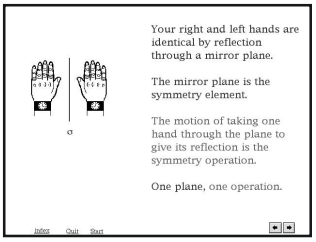
Crystallography Collection

Point Group I, II, and III



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Point Group I, II, and III is a series of programs for Mac OS and Windows designed to teach point group symmetry. The complete package of instructional programs and exercises is appropriate for upper-division undergraduate or graduate courses in inorganic or physical chemistry. The first two units can be used at whatever level symmetry elements are introduced. They were written for a sophomore inorganic chemistry course that follows an organic chemistry course taken in the first year.

Contents

Point Group I: Introduction to Point Group Symmetry Elements and Operations is a detailed presentation using images of hands and ethane in staggered and eclipsed conformations to describe the symmetry. This unit takes students approximately 45 minutes to complete. Color coding is used to help students learn the difference between symmetry elements (blue symbols and words) and symmetry operations (red symbols and words).

Point Group II: Counting Symmetry Elements provides an interactive template wherein the user enters the number of each symmetry element found in a species. When finished, the user can check the answers. The program indicates any errors and includes hints for common errors to assist the user. Users should have molecular models in hand. Three sample programs are included. The first is suitable for use with students who have a general chemistry-level understanding of VSEPR; the second assumes understanding of transition-metal complexes and isomerization; the third makes use of 3D models of works by Escher (*1*). A "Teacher Template" is included that allows the instructor to make custom-designed units using any species of chemical interest.

Point Group III: Point Group Nomenclature presents the user with a "decision tree" for assigning the name of the point group for a species. If the incorrect name is selected, the program indicates the branch in the tree where the wrong path was taken. Three sample programs using the same species as in the Point Group II sample programs are provided.

Table 1. Hardware and Software Required for Point Group I, II, and III

Computer	CPU	RAM	Drives	Free Disk Space	Graphics	System	Other Software
Mac OS Compatible	PowerPC	≥ 24 MB	CD-ROM; Hard disk	20 MB	≥ 640 × 480; thousands or millions of colors	System 7.6.1 or higher	QuickTime 4; HyperCard Player
Windows Compatible	80486 or higher	≥ 24 MB	CD-ROM; Hard disk	36 MB	≥ 640 × 480; 16-bit or 24-bit color	Windows 98/95	QuickTime 4

A program for the instructor to generate a custom-designed unit is also included.

How to Use Point Group I, II, and III

Point Group I, II, and III have been used by the author in a student-centered instructional setting, where students use the programs and the instructor is available to help as required; and for independent study, with the instructor meeting with the students between units to clarify material as needed. Individual units can be employed in other settings. Although this package is intended for individual use, a few examples suitable for projection are included in Point Group I.

Hardware and Software Requirements

Hardware and software requirements for Point Group I, II, and III are found in Table 1. Point Group I, II, and III were created using Macromedia Director (*2*), QuickTime (*3*), Toolbook (*4*) (for the Windows version), and HyperCard (*5*) (for the Mac OS version).

Acknowledgments

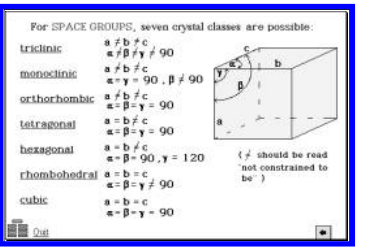
Point Group I, II, and III were produced with support by the Camille and Henry Dreyfus Foundation, Inc. (1997–1999).

Literature Cited

1. Schattschneider, D.; Walker, W. *M. C. Escher Kaleidocycles,* revised ed.; Pomegranate Communications: Rohnert Park, CA, 1987.
2. Macromedia Director, version 6.5; Macromedia, Inc.: San Francisco, CA, 1998.
3. QuickTime, version 3.0; Apple Computer: Cupertino, CA, 1998.
4. ToolBook II, Instructor, version 6.0; Asymetrix: Bellevue, WA, 1998.
5. HyperCard 2.3.5; Apple Computer: Cupertino, CA, 1998.

Crystallography Collection

Crystallographic CourseWare



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Crystallographic CourseWare is a series of modules for Mac OS and Windows designed to teach fundamental concepts in crystallography. The complete package of instructional programs and exercises is intended for use in an upper-division undergraduate or graduate special-topics course. Individual units can be used in general, inorganic, or physical chemistry courses.

Contents

Crystallographic CourseWare contains 12 modules.

1. **Crystal Growth** includes text and animation describing how to grow crystallographic-quality crystals.
2. **Symmetry** provides definitions, illustrations, and animations of symmetry elements and operations typically observed in triclinic, monoclinic, or orthorhombic unit cells.
3. **More Symmetry** extends the information in Symmetry to include less common symmetry such as diamond glides, and 3_n and 6_n screws; includes a comparison of S_6 and $\overline{3}$ symmetry operations.
4. **Unit Cells and Asymmetric Units** has definitions, illustrations, and animations including both plane group and space group lattices.
5. **Exercises in Plane Group Symmetry** provides a simple drawing toolbox for students to locate and identify the location of plane group symmetry elements, the unit cell, and asymmetric unit for a simple motif illustrating each of the 17 plane groups; additional exercises include motifs located at special positions. Answers are available on-screen for all exercises, with animations detailing how the answer is found in the pattern for some. Two of the animations extend the instruction to introduce the standard symbols used in the *International Tables for Crystallography* (*1*) and general positions.
6. **Exercises in Reading the *International Tables for Crystallography*** provides a simple drawing toolbox for students to build an understanding of the relationships between general positions (*x*, *y*, *z*), symmetry elements, and general position projections as presented in the *International Tables for Crystallography*. Some examples have answers included, others can be found in the *Brief Teaching Edition of the International Tables for Crystallography* (*2*), and the rest require access to the complete *Tables* and thus can be used as quiz materials.
7. **Reciprocal Space** provides a step-by-step illustration of the relationship between real and reciprocal lattices, with an introduction to systematic absences as might be seen in precession photographs or computer-generated images of the reciprocal lattice.
8. **Precession Photographs** provides instruction with simple exercises for the indexing of precession photographs and further instruction on how to identify systematic absences and use that information to identify possible space groups.

Table 2. Hardware and Software Required for Crystallographic CourseWare

Computer	CPU	RAM	Drives	Free Disk Space	Graphics	System	Other Software
Mac OS Compatible	PowerPC	≥ 24 MB	CD-ROM; Hard disk	38 MB	≥ 640 × 480; thousands or millions of colors	System 7.6.1 or higher	QuickTime 4; HyperCard Player
Windows Compatible	80486 or higher	≥ 24 MB	CD-ROM; Hard disk	83 MB	≥ 640 × 480; 16-bit or 24-bit color	Windows 98/95	QuickTime 4

9. **Scattering Factors** contains interactive programs to allow users to observe the change in scattering power as a function of the angle of scattering, the radiation source used, the atoms causing the scattering, and thermal motion.
10. **Thermal Parameters** provides instruction to allow recognition of well- or poorly-behaved molecules by looking at the thermal ellipsoid plots. The Windows version also includes interactive programs for students to explore the relationship between the algebraic and graphical representations of ellipses.
11. **Fractional Crystal Coordinates** (Windows only) provides interactive exercises to assist students in learning how the fractional crystal coordinates relate to the position of molecules in the unit cell, how the general positions correspond to the placement of replicate molecules within the cell, and how the general position projection diagrams as given in the *International Tables for Crystallography* (*1*) would change in appearance if the magnitude of *x*, *y*, and *z* were changed.
12. **Special Positions** (Windows only) provides interactive exercises requiring the user to identify all of the point group symmetry elements in a species, identify the point group using a typical flow diagram, and identify the possible special position locations of molecules using the symmetry projection diagrams as provided in the *International Tables* (*1*).

How to Use Crystallographic CourseWare

Crystallographic CourseWare has been used in a student-centered (*3*) instructional setting, with students using the programs and the instructor available to help students as required; and for independent study, with the instructor meeting with the students between units to clarify material as needed. Individual units can be employed in other settings. For example, the instructional units on two-dimensional symmetry, unit cells, and asymmetric units and the related exercises can be used in a general chemistry course, particularly for engineering students who will subsequently be taking a materials science course. The unit on crystal growth can be effectively used by students doing synthetic research where one goal is the growth of crystallographic-quality crystals. The units on reciprocal space and precession photography could be used in physical chemistry courses. Although designed for individual or group student use, some units could be projected for use in lecture courses.

Well-prepared and motivated students can use Crystallographic CourseWare together with a standard text to make substantial progress learning crystallography in an independent-study course. The programs do not eliminate the need for the instructor, but they do allow the time spent one-on-one to be directed at clarification of issues rather than basic instruction. A syllabus used by the instructor for students doing a "half-course" or a "full-course" using a combination of these programs, a standard text, live demonstrations, and other exercises is provided in the documentation.

Hardware and Software Requirements

Hardware and software requirements for Crystallographic CourseWare are found in Table 2. Crystallographic CourseWare was created using Macromedia Director (*4*), QuickTime (*5*), Toolbook (*6*) (for the Windows version), and HyperCard (*7*) (for the Mac OS version).

Acknowledgments

Crystallographic CourseWare has been in production for ten years. Various parts of it have been class tested as described in the "How to Use…" section above and the patience and comments of those students is appreciated. Also greatly appreciated are the comments of peer reviewers of the software, both formal and informal.

The HyperCard version and related QuickTime movies were produced with support from the Pew Charitable Trusts as administered through the Mid-Atlantic Cluster (1991–1992). The ToolBook version and cross-platform Macromedia Director units were produced with support by the Camille and Henry Dreyfus Foundation, Inc. (1997–1999).

Literature Cited

1. *International Tables for Crystallography: Volume A: Space Group Symmetry*; Hanh, T., Ed.; D. Reidel: Boston, 1983.
2. *International Tables for Crystallography, Brief Teaching Edition of Volume A, Space-Group Symmetry,* 3rd ed.; Hanh, T., Ed.; Dordrecht: Boston, 1993.
3. Kastner, M. E. *J. Appl. Crystallogr.* **1999,** *32*, 327–331.
4. Macromedia Director, version 6.5; Macromedia, Inc., San Francisco, CA; 1998.
5. QuickTime, version 3.0; Apple Computer: Cupertino, CA, 1998.
6. ToolBook II, Instructor, version 6.0; Asymetrix: Bellevue, WA, 1998.
7. HyperCard 2.3.5; Apple Computer: Cupertino, CA, 1998.