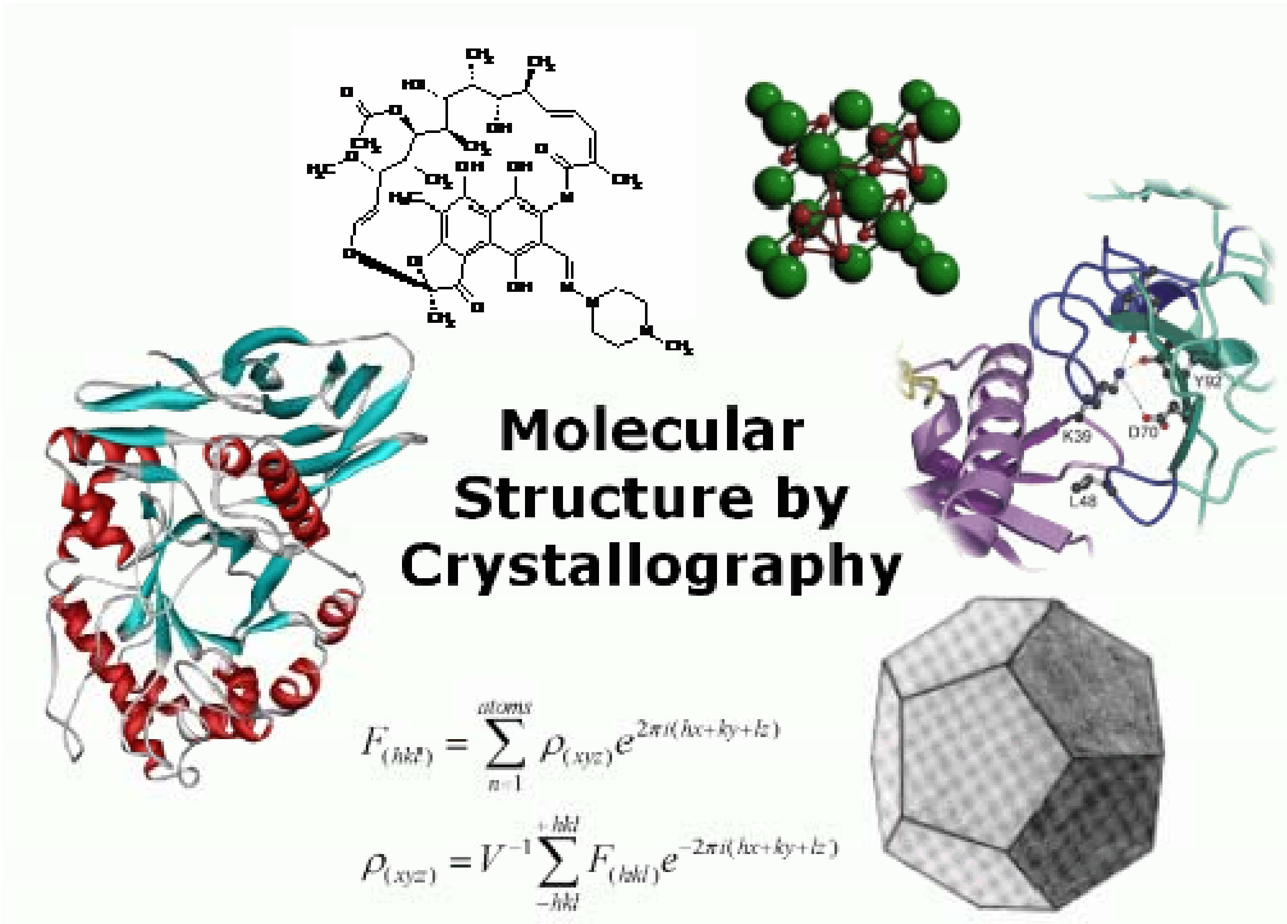


Crystallography Education Policies for the Physical and Life Sciences

Sustaining the Science of Molecular Structure in the 21st Century

Prepared by the American Crystallographic Association
and the United States National Committee for Crystallography

Preface

In 2001 and 2003, the United States National Committee for Crystallography (USNC/Cr) Education Subcommittee conducted two surveys (Appendix B). The first survey aimed to determine the content and extent of coverage of crystallography in university curricula, while the second solicited the views of the broader crystallographic community on the status of crystallography education and training in the US, in both the physical and the life sciences. *The results of these surveys suggested that, perhaps due to rapid technological advances in the field of modern crystallography, there appears to be a declining number of professional crystallographers, as well as a lack of sufficient education and training in crystallography for individuals who wish to understand and/or use crystallography in their hypothesis-driven research*. Recognizing the opportunity to communicate to the broader scientific community the research opportunities afforded by crystallography, as well as the value of crystallographic information, the education committees of the American Crystallographic Association (ACA) and USNC/Cr organized a crystallography education summit, which took place June 1-2, 2005 at the conclusion of the ACA national meeting in Orlando, FL. A broad range of individuals known for their experience and contributions in crystallography education and training participated in this summit (Appendix A). The outcome of this process is this consensus policy statement on crystallography education and training.

The ACA is a non-profit, scientific organization of nearly 2200 members, founded in 1949 as a merger of the American Society for X-ray and Electron Diffraction and the Crystallographic Society of America. The objective of the ACA is to promote interactions among scientists who study the structure of matter at atomic or near atomic resolution. These interactions will advance experimental and computational aspects of crystallography and diffraction, as well as promote the study of the arrangements of atoms and molecules in matter and the nature of the forces that both control and result from these arrangements. The ACA is the primary professional organization for crystallographers in the US and the regional affiliate to the International Union of Crystallography (IUCr). The standing committees of the ACA Council include Communications, Data Standards and Computing, and Continuing Education.

The USNC/Cr represents US crystallographers in the IUCr under the auspices of the National Academies' National Research Council. The USNC/Cr promotes the advancement of the science of crystallography in the United States and throughout the world. Crystallographic information is key for a variety of fields in biological and physical sciences. By representing the broad US crystallographic community, the USNC/Cr also serves a unique role in bringing together crystallographers in the areas of biochemistry, structural biology, pharmaceuticals, materials research (including crystalline and non-crystalline materials), surface studies, mineralogy, inorganic chemistry, powder diffraction, crystal growth and crystallography education. The USNC/Cr supports activities and addresses issues in interdisciplinary research, research resources and facilities, education and travel support, crystallographic databases, and publication standards and ethics. Its role is increasingly important for maintaining a high level of professionalism in a community that spans many disciplines and professional societies, and that needs international communication and coordination.

Acknowledgements

This policy document is the product of many people. First, we thank those members of the USNC/Cr Education Subcommittees who began reviewing the status of education and training in crystallography and who administered the original surveys (listed alphabetically): Ray Davis, University of Texas Austin; Frank Fronczek, Louisiana State University; Katherine Kantardjieff, California State University Fullerton; Cheryl Klein Stevens, Xavier University; Ian Robinson, University of Illinois at Urbana-Champaign; Cynthia Stauffacher, Purdue University. We also thank Charles Carter, University of North Carolina Chapel Hill, past president of the ACA, and Marvin Hackert, University of Texas Austin, past chair of the USNC/Cr, for their support and inspiration.

Second, we thank the summit participants (listed alphabetically), whose biographical information is given in Appendix A: Robert Bau, University of Southern California; Simon Billinge, Michigan State University; Gloria Borgstahl, Eppley Institute, University of Nebraska; Charles Campana, Bruker-Nonius Analytical X-ray Systems; Jon Clardy, Harvard Medical School; Frank Fronczek, Louisiana State University; Andy Howard, Illinois Institute of Technology; Allen Hunter, Youngstown State University; Frances Jurnak, University of California Irvine; James Kaduk, Innovene; Katherine Kantardjieff, California State University Fullerton; Margaret Kastner, Bucknell University; Cheryl Klein Stevens, Xavier University; Marilyn Olmstead, University of California Davis; James Pflugrath, Rigaku MSC; Kent Ratajeski, University of West Georgia; Miriam Rossi, Vassar College; Bernhard Rupp, University of California-Lawrence Livermore National Laboratory; Robert Sweet, National Synchrotron Light Source; Iris Torriani, University of Campinas, Brazil; and Victor Young, University of Minnesota.

Third, we thank Elaine McClanahan from Strategic Learning, who facilitated the summit, and Dr. Jerry Bell of the American Chemical Society for his motivating keynote address. We also thank members of the ACA Continuing Education Committee and the USNC/Cr Education Subcommittee who helped organize the summit and who served as facilitators during break-out sessions (listed alphabetically): Simon Billinge, Gloria Borgstahl, Frank Fronczek, Frances Jurnak, Katherine Kantardjieff, Cheryl Klein Stevens, Marilyn Olmstead, and Miriam Rossi. Thanks to Bernhard Rupp for his cover design, and to Andy Howard for his integrated figure on page 15.

Finally, we wish to thank those organizations who generously provided financial support for this summit: the United States National Committee for Crystallography, the American Crystallographic Association, the National Science Foundation, and the California Program for Education and Research in Biotechnology.

Executive Summary

Practically all information about the molecular structure of matter at atomic resolution is the result of crystallographic analysis, using data obtained by X-ray, neutron and electron diffraction methods. Diffraction methods have contributed to our fundamental understanding of chemical bonds, chemical reactions and biochemical pathways, the composition and properties of minerals and ceramics, and to the design of materials, pharmaceuticals, crystals, and enzymes. Methodological advances in the past 30 years provide opportunities for individuals with diverse backgrounds and preparation to use crystallography to answer structural problems in their hypothesis-driven research. These same technical advances now enable users with little or no training (or deeper understanding) to often (but not always) produce quality results.

> *"Crystallography borders, naturally, on pure physics, chemistry, biology, mineralogy, technology and also on mathematics, but is distinguished by being concerned with the methods and results of investigating the arrangement of atoms in matter, particularly when that arrangement has regular features."*
>
> \- ***Paul Ewald***
> *Acta Crystallographica 1 (1948) 2*

The rich and interdisciplinary science of crystallography was described eloquently by Paul Ewald in 1948 (see insert). This statement is still true today, and it is with his philosophy that the present document is written. Modern crystallography provides enabling technology, methodology and information, and *the bounty of knowledge gained from analysis of its structures is a key underpinning of modern science and technology*. There is common ground in the fundamental physics of crystallography shared by scientists in the life sciences and by those in the physical sciences, but the objectives of each community in applying crystallography to their particular research problems are not necessarily the same. Life scientists are generally interested in overcoming the modern-day bottlenecks of crystallization and protein production, and in learning the basic requirements to use crystallographic techniques, namely data collection and executing various software applications that determine molecular structures in a nearly automated fashion. Physical scientists, particularly those from the fields of inorganic chemistry and materials science, are often concerned about fundamental symmetry, space groups and unit cells, which give rise to the material and reactive properties of the crystalline state. These topics naturally require greater depth of understanding of the underlying crystallographic principles. The life science and physical science communities can be further divided into two major categories: ***professional crystallographers*** and **users/consumers** of crystallography. **Professional crystallographers** are experts who devote a majority of their research efforts to implementing and developing crystallography, and who require both depth and breadth of knowledge, as well as hands-on experience. ***Users*** of crystallography employ, but do not develop crystallographic methods. Nonetheless, they require a sufficient working knowledge of the field that enables them to answer specific research questions and to collaborate with those having greater expertise. ***Consumers*** of crystallographic information – with similar educational needs as ***Users*** - include theoreticians, bioinformatics scientists, pharmaceutical scientists, chemists or materials scientists, who utilize crystallographic results as the basis for or validation of their own work. Consumers do not conduct crystallographic analysis, but need to understand crystallographic notations and basic symmetry for interpretation and judgment of the quality of crystallographic results to avoid over- and mis-interpretation.

Organization and Content This document summarizes the crystallography education and training policies endorsed by the ACA and the USNC/Cr. Organized in a reverse hierarchal order, beginning with post-baccalaureate education and working back to the K-12 level, this policy document makes recommendations for a comprehensive re-evaluation of crystallography education, and it suggests ways to develop in the broader scientific community an appreciation for the value of crystallographic information. Moreover, the visual, aesthetic and quantitative nature of crystallography – as exemplified by the cover graphics - provides an excellent path to introduce science and scientific methods to the general population. The conclusions and recommendations in this document are based on input from the education summit participants: biologists, biochemists, chemists, geologists and physicists, all practicing crystallographers in their fields, representing both academia and industry (Appendix A).

Intended Audience and Desired Outcomes These draft policies are directed towards our scientific colleagues, who may also be practicing crystallographers, as well as education policy makers of the major scientific societies. It is the hope of the ACA and the USNC/Cr that this document, which stands as the white paper on crystallography education and training for the 21st century, provides guidelines to professional societies, academic departments, and funding agencies for crafting future crystallography curricula that adequately address the needs of the entire scientific community. The Continuing Education Committee of the ACA and the USNC/Cr Education Subcommittee will provide guidance and support to interested colleagues and policy makers who wish to put these recommendations into practice.

In creating this document, the summit participants have recognized that

- crystallography and molecular structure awareness should begin in K-12 education as core components for implementing the established national science standards for all students
- many contexts exist in which crystallography can be incorporated in undergraduate education with minimal disruption to current courses, and should be included in curricula of all undergraduate programs in the physical and life sciences
- formal courses and research opportunities in crystallography should be available to senior undergraduates
- crystallography-rich courses should be available to all graduate students
- professional development beyond the graduate degree, such as provided by crystallography certificate programs, short courses, summer schools and research opportunities, is a necessary aspect of crystallography training; this is particularly important in novel subjects such as modulated structures and time-resolved diffraction, where crystallography is increasingly being outsourced
- the recommendations made and resulting changes effected must benefit the broader scientific community and not just the community of professional crystallographers

> *"The hallmarks of a crystallographer in the 21st century will be his/her skillful analysis of structures in chemical, biological or geological context, knowledge of material preparation and synthetic methods, and a solid repertoire of techniques tailored to the increasingly challenging structural problems in contemporary science."*
>
> - ***K. Kantardjieff and B. Rupp***
> *Zeischrift für Kristallographie 7 (2002) 328*

If the science of crystallography is to remain alive and vibrant, it is critical that crystallography be taught in a way that attracts and retains a broad pool of talented people. Although the United States has played a prominent role in technological and scientific advancement, there has been a recent, faltering interest and diminished academic performance in math and science by American students. Crystallography, with its interdisciplinary nature and diversity of practitioners and users, provides a prime opportunity to reinvigorate interest in science, to attract and maintain an important share of scientific talent. Maintaining the vitality of crystallography is important to university departments advancing science. Education and training today will contribute to the production of a successful workforce that will assist the nation to prosper in a world of global economic competition.

Post-Baccalaureate Education and Professional Development

Post-Baccalaureate Education This includes programs at the graduate certificate, Masters (MS) and the doctoral (PhD) formal levels of education and, for those pursuing academic positions or project management positions in industry, a post-doctoral experience. Given the high impact and rapid pace of methods development in crystallography, there is ample reason, *and opportunity*, to advertise the importance of studying crystallography to all science graduates. While there is common ground in the fundamental physics of crystallography between those in the life sciences and those in the physical sciences, the objectives of these communities in applying crystallography to their particular research problems are not necessarily the same, and each community can be divided into professional crystallographers and users/consumers of crystallographic information. Professional crystallographers are frequently consulted on difficult problems which require depth of knowledge and expertise; they develop new and more sophisticated methods, algorithms and automation, and engage the most challenging structures. User crystallographers require a sufficient working knowledge of the field to answer specific research questions, and a support infrastructure including collaborations with those having greater expertise.

Post-doctoral staff scientist Brian Schick aligns a protein crystal sample on a 4-circle goniostat.

With the migration of academic crystallography from a research specialty to a technique employed by a wide community of users, few university departments hire faculty capable of teaching crystallography, and representation of crystallography in university curricula has diminished markedly over the last decade. At this same time, its employment by increasingly large numbers of inadequately trained and supported users has rapidly accelerated. This has led to an increasing reliance on other, non-curricular resources, such as web pages, which allow crystallography to be self-taught. While web-based tutorials are often well-constructed and can provide an extremely valuable resource to the broader scientific community, such tutorials can not take the place of practical experience, nor do they transmit the fascination and excitement in the field that will interest a future generation of professional crystallographers. Although education at the graduate level continues to stress original, basic research and development of problem-solving skills of its students, crystallography, as an interdisciplinary science with a tradition of having diversity among its practitioners and users, affords the opportunity to help students recognize the broader applicability of their skills.

Professional Development Given the high impact and rapid pace of methods development in crystallography, individuals will often seek continuing education opportunities to hone their skills, learn new ones, or perhaps change research direction, all of which require acquisition of new knowledge and skills. The American Crystallographic Association and other professional scientific organizations impacted by crystallographic science must continue to embrace opportunities to sponsor or support educational activities that will benefit crystallographers, scientists and educators. In addition, these organizations should promote diversity by educating persons traditionally underrepresented in the sciences. These activities may involve the entire crystallographic community or a portion of it. Continuing education and professional development activities, which may be conducted as schools, workshops or courses, generally fall into three categories:

Structure validation workshop held at the ACA national meeting in Orlando, FL 2005.

- continuing education aimed at experienced crystallographers to enhance and update their competence
- professional development opportunities aimed at scientists wishing to learn about and use crystallography in their research, and for individuals seeking retraining for new careers
- education outreach aimed at faculty, teachers and students to provide information about teaching crystallography in secondary schools, as well as undergraduate and graduate programs

To be effective, these schools, workshops and courses should have a statement of purpose and desired outcomes, a statement describing the benefits to the crystallographic community and/or the broader scientific or education community, and assessment metrics. Following the recommendations outlined below, the content should be tailored and scheduled to meet the needs of the intended audience. Whenever possible and appropriate, industrial participation and sponsorship should be encouraged.

Recommendations for the Professional Crystallographer in the Life Sciences

1. ***Intellectual Context***
   a. A professional crystallographer in the life sciences should be able to recognize and appreciate the synergy between crystallography and related techniques.
   b. A professional crystallographer should appreciate the information content of experimentally derived biomolecular structures and their limitations.
2. ***Advanced Concepts and Applications***
   a. A professional crystallographer should recognize and appreciate the potential of structural genomics, protein engineering, drug discovery and bioinformatics.
   b. A practitioner should stay current, and even anticipate and participate in developments.
3. ***Molecular Concepts***
   a. A professional crystallographer should fully understand molecular structure, including bonds, angles, stereo-chemistry and non-covalent interactions.
   b. In addition, a professional crystallographer should understand basic biochemistry, including transcription and translation, enzyme kinetics, thermodynamics, protein-ligand interactions, and the roles of water and metals in structure and function.
4. ***Crystallization and Sample Preparation***
   a. A professional crystallographer in the life sciences should understand and be able to apply methods of protein expression, purification, production, and the chemical/biochemical methods of protein labeling.
   b. Furthermore, such a professional crystallographer should understand and be able to apply principles of crystal growth, including super-saturation, kinetics of crystal nucleation and growth, crystal growth methods, and crystal stability (osmolality, ionic strength, pH).
5. ***Computational Methods, Data Use and Model Evaluation***
   a. A professional crystallographer should understand and be able to apply methods of phase determination, including heavy atom refinement, Multiple Anomalous Dispersion (MAD) techniques, Molecular Replacement, Direct Methods, Density Modification and Non-Crystallographic Symmetry (NCS) averaging.
   b. A professional crystallographer should be competent in model building, phase bias removal, refinement methods, structure validation, and the use of bioinformatics tools.

6. Mathematics

a. A solid understanding of Fourier mathematics, least-squares and maximum likelihood, error propagation and statistics, and precision vs. accuracy (see also under professional crystallographer in Physical sciences) is essential to the professional crystallographer.

7. Practical Knowledge and Skills

a. A professional crystallographer must be proficient in the use of computers as his/her essential tool, which should include knowledge of operating systems and programming skills.

b. A professional crystallographer must be able to troubleshoot instrumentation and optimize X-ray beam characteristics to suit a particular experiment, including sources of background, beam collimation, and monochromatization.

c. A professional crystallographer must demonstrate an ability to perform necessary experimental procedures, such as cryo-mounting, selecting a data collection strategy, data reduction and sample characterization (effective mosaicity, diffraction limit)

d. A professional crystallographer should be able to communicate crystallographic results and methods to specialists, non-specialists, and non-scientists.

The Laboratório Nacional de Luz Sincrotron (LNLS) in Campinas, Brazil.

8. Crystal Physics and the Solid State

a. A professional crystallographer should have an understanding of the physical properties of crystals and their origins (mosaic spread, flash cooling, and phase transitions).

9. Diffraction Physics

a. A professional crystallographer should understand anisotropy of sample ordering and absorption, radiation damage, contrast variation/deuterization, resolution and sinθ-dependent properties, and internal functions of data reduction (indexing, profile fitting, scaling).

10. Geometry of Diffraction and Symmetry

a. A professional crystallographer should understand Bragg's Law, the reciprocal lattice and the Ewald construction, unit cells and the asymmetric unit, space groups and the implications of symmetry (absences), as well as non-crystallographic symmetry.

11. Basic Physics

a. A professional crystallographer should understand Thomson scattering, coherence length, beam polarization, and anomalous scattering (fluorescence, absorption, Δf', Δf", Kramers-Kronig transform), as well as the nature of X-ray optics (cross-fire, bandwidth) and the production of X-rays (laboratory sources vs. synchrotron).

Recommendations for the User of Crystallography in the Life Sciences Requiring a Working Knowledge of the Field

1. Intellectual Context

a. A user of crystallographic methods and tools appreciates the extraordinary wealth of information provided by structural biology and the impact of crystallography on life sciences.

2. Crystallization and Sample Preparation

a. A user understands the process of sample preparation, quality and quantity as needed for the objective of the biophysical application.

3. Basic Concepts

a. A user understands the concepts (e.g., diffraction, statistics, bonding, intermolecular interactions) necessary to appreciate the powerful results, as well as the advantages and limitations of the method.

b. A user has a qualitative understanding of the interaction of electromagnetic waves with periodic arrays, diffraction and reconstruction to form an electron density image.

Graduate student James Ongaro cryo-mounts crystal samples for the synchrotron beam line.

4. Computational Methods, Data Use and Evaluation of Results

a. Competent users of X-ray models will be able to obtain, view, interpret, and evaluate them confidently.

5. Advanced Concepts and Applications

a. A user of crystallography methods and tools appreciates the technical aspects involved in a crystal structure determination, and how these aspects can influence the final results (e.g. that default parameters established by software are not always appropriate).

6. Molecular Concepts

a. To communicate and use molecular concepts in their own research, users will understand the fundamentals of three-dimensional structure e.g., proteins, ligands, macromolecular structure, and structural motifs.

b. Users will understand how proteins interact dynamically at the molecular level with other proteins, nucleic acids, small molecules, drugs and substrates.

7. ***Practical Knowledge and Skills***
   a. An understanding of the capabilities and challenges of the crystallographic process will enable users to develop their own realistic structural studies and collaborations.

Recommendations for the Professional Crystallographer in the Physical Sciences

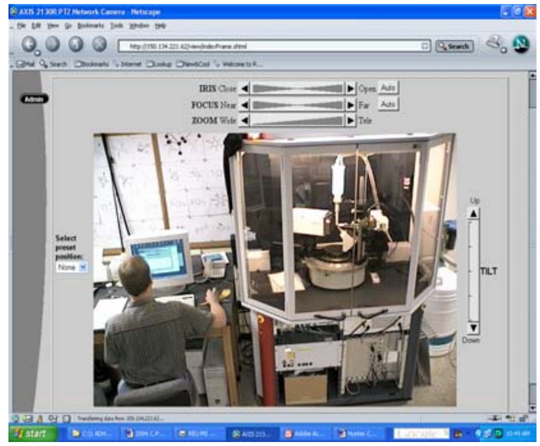
1. ***X-rays and Diffraction Physics***
   a. A professional crystallographer will understand the physics of the generation of X-rays, electrons and neutrons, scattering phenomena, and how they are related to molecular structure.
   b. A professional crystallographer will understand the relative advantages and applicability of X-rays versus neutrons versus electrons for different types of studies.
2. ***Crystallization and Sample Preparation***
   a. A professional crystallographer will be able to obtain appropriate material for study, choose and optimize crystallization conditions, select suitable crystalline specimens, and will be familiar with techniques to handle unstable samples.
3. ***Crystal Physics and the Solid State***
   a. A professional crystallographer will understand the nature of the solid state and its relationship to properties, including phase transitions, twinning and other imperfections.
   b. A professional crystallographer will understand solvent properties, solute-solvent interactions, and the crystal growth process to guide crystallization studies.
4. ***Geometry of Diffraction and Symmetry***
   a. A professional crystallographer should understand Bragg's Law, the reciprocal lattice and the Ewald construction, unit cells and the asymmetric unit.
   b. A professional crystallographer will understand group theory, sub- and super groups/structures and their relationship to phase transitions, point and space groups and the implications of symmetry (absences), as well as non-crystallographic symmetry, and how local structure may deviate from long-range ordering.
5. ***Mathematics***
   a. A solid understanding of Fourier mathematics, least-squares and maximum likelihood, error propagation and statistics, and precision vs. accuracy, is essential to the professional crystallographer.
6. ***Basic Physics***
   a. An understanding of Thomson scattering, coherence length, beam polarization, and anomalous scattering (fluorescence, absorption, $\Delta f'$, $\Delta f''$, Kramers-Krönig transform) is essential to the professional crystallographer.

b. An understanding of the nature of X-ray optics and the production of X-rays (laboratory sources and synchrotron) is required of the professional crystallographer.

7. Instrumentation

a. A professional crystallographer will have an applied knowledge of laboratory-based X-ray diffraction instrumentation and its function, as well as interfacing with computers and networks.

b. A professional crystallographer will be able to apply experimental techniques and collect measurements requiring user facilities, such as synchrotrons.



Post-doctoral staff scientist Matthias Zeller collects low temperature data on a laboratory CCD diffractometer system.

8. Advanced Concepts and Applications

a. A professional crystallographer appreciates and understands advances in the modeling of non-routine structural problems, including the concept of chirality and methods of determining absolute structure, and of treating complex structures such as those involving supercells and twinning.

b. A professional crystallographer understands and appreciates the capabilities and limitations of powder diffraction crystallography and Rietveld refinement.

c. A professional crystallographer will understand and use quantum mechanical and other computational tools as a key part of doing contemporary crystallography.

9. Molecular Concepts

a. A professional crystallographer is able to interpret the results of the experiment and translate these results into an understanding of chemical bonding, packing, and other properties.

10. Practical Knowledge and Skills

a. A professional crystallographer should have a developed skill set that includes the use of advanced instrumentation, software packages and databases, presentation of results, and 3-D visualization.

b. A professional crystallographer should be able to communicate crystallographic results and methods both to specialists, non-specialists and non-scientists.

11. ***Computational Methods, Data Use and Evaluation of Results***
    a. A professional crystallographer should understand and be able to apply methods of phase determination and refinement, including Direct Methods and Patterson Methods.
    b. A professional crystallographer will be able to confidently apply validation tools and statistics, understand the accuracy and relevance of results, and access and contribute to crystallographic databases.

Recommendations for the User Crystallographer in the Physical Sciences Requiring a Working Knowledge of the Field

1. ***Intellectual Context***
    a. As a consumer of crystallographic information, a user should understand the origin, interpretation, uses, and limits of crystallographic studies.
2. ***Crystals and the Solid State***
    a. A user should understand the nature of the solid state, the types of solid state structures, and their relationship to solution and gas phase structures.
3. ***Advanced Concepts and Applications***
    a. A user should have an initial exposure to advanced topics such as charge density diffraction, neutron methods, macromolecular crystallography, twinned crystals, etc.
4. ***Crystallization and Sample Preparation***
    a. A user should understand how to prepare and select crystalline samples, and evaluate their suitability for diffraction studies.
5. ***Computational Methods, Use of Data and Evaluation of Results***
    a. A user should understand crystallography terminology reported in the literature and be able to critically evaluate the results presented.
    b. A consumer of crystallographic information should be able to critically analyze crystallographic results to evaluate their reliability and utility.
    c. Consumers of crystallographic information should be aware that although many structures can now be solved by individuals with little understanding of crystallography, avoidance of significant, but subtle, errors requires an awareness of the multiple difficulties that can occur.

Two-Year Colleges, Four-Year Colleges and Universities

Practically all information about the molecular structure of matter at atomic resolution is the result of crystallographic analysis. Diffraction methods have contributed to our fundamental understanding of biochemical pathways and chemical reactions, the composition and properties of minerals and ceramics, and to the design of material properties, pharmaceuticals and engineered enzymes. It is essential that undergraduates understand and appreciate the origins of molecular structural information and the biological, chemical and physical implications derived from this information. Moreover, crystallography is an ideal topic for faculty to embrace and include within the context of their undergraduate courses in life and physical sciences. Crystallography underscores the importance of interdisciplinary science and, by directly and tangibly affecting all our lives through advances in biosciences up to space-age high tech materials development, crystallography can excite and stimulate a broad spectrum of students.

Community Colleges The nation's 1150 two-year or community colleges (CCs) provide access to careers in science, engineering and technology for more than 10 million students, particularly students traditionally underrepresented in the sciences. Students attending two-year colleges prepare for jobs as technicians in industry, academia and government, as well as for transfer to baccalaureate programs at four-year colleges and universities. It is, therefore, equally important that students taking preparatory or general education science courses at two-year colleges develop an appreciation for the origins of molecular structural information and the biological, chemical and physical implications derived from this information. Faculty at community colleges, who typically carry heavy teaching loads, should be given opportunities for continuing education in crystallography to ensure that students are exposed to contemporary concepts in a stimulating way.

Students in a senior biochemistry laboratory prepare crystallization screening experiments for chicken muscle lactate dehydrogenase.

Predominantly Undergraduate Institutions Despite their sometimes relatively small science programs, predominantly undergraduate institutions (PUIs) excel at attracting good students to science and encouraging them to enter graduate programs. Indeed, PUIs have a leading role in undergraduate education by providing the majority of BS graduates who go on to do a PhD in the sciences. Along with CCs, they provide the primary pathway for recruiting the next generation of professional scientists in general, and crystallographers in specific, into professional careers. Although undergraduate research is recognized as an effective strategy for teaching and refining skills, faculty at PUIs are often challenged to conduct and maintain productive contemporary research programs by constraints on time and resources. It is to the benefit of the broader scientific community that PUI faculty members are supported in their efforts to integrate crystallographic

Graduate student Abdul-Basis Alhassan and undergraduate Jennifer Patton discuss sample mounting.

topics into their teaching, and crystallographic methods into their research. Moreover, it is in the personal best interests of professional crystallographers and their institutions, funding agencies, and the nation to ensure that adequate support is in place to fully integrate crystallography into undergraduate teaching and research.

Recommendations for Undergraduate Students in the Life Sciences

1. ***Intellectual Context***
   a. An undergraduate student will appreciate the extraordinary wealth of information provided by structural biology and the impact of crystallography on life sciences.
2. ***Basic Concepts of X-rays and Scattering***
   a. An undergraduate will have a qualitative understanding of the interaction of electromagnetic waves with periodic arrays, diffraction and reconstruction to form an electron density image, symmetry in nature and its use in the assembly of macromolecules.
   b. An undergraduate student will understand the advantages and limitations of diffraction.
3. ***Data Usage and Model Evaluation***
   a. All competent users of X-ray models will be able to obtain and view them from appropriate databases and extract useful information from them (e.g. active site residues, secondary and tertiary structure, etc). More advanced users should have detailed knowledge of the contents of these databases.
4. ***Molecular Concepts***
   a. Undergraduates should have a solid understanding of the fundamentals of three-dimensional structure in order to communicate and use these concepts in the context of other courses in the curriculum and in their own inquiry and investigation.
   b. The function of the macromolecule is determined by the 3D arrangement of the atoms.
   c. Biomolecular structures derived from crystallographic analysis should be used to develop students' understanding of protein interaction at the molecular level with other proteins, nucleic acids, small molecules, drugs, and substrates.
5. ***Advanced Concepts and Applications***
   a. Biomolecular structure provides the molecular basis of human health and disease.
   b. The results of protein crystallographic analysis may be used to further develop students' understanding of the molecular basis of heredity and biological evolution, as well as matter, energy and organization of living systems.

Recommendations for Undergraduate Students in the Physical Sciences

1. ***Intellectual Context***
   a. Students will develop an appreciation for the technique, vocabulary and applications of X-ray diffraction.
2. ***Basic Concepts of X-rays and Scattering***
   a. Students will develop an appreciation for the nature, production, and scattering of X-rays.
3. ***Instrumentation***
   a. Students will develop a basic understanding of diffraction instrumentation at a similar level to that taught for other key instruments such as nuclear magnetic resonance spectrometers, infrared spectrometers, gas chromatography or high-performance liquid chromatography systems.
4. ***Crystals and Crystallization***
   a. Students will understand the basic properties of crystals including crystal growth, defects, and quality.
5. ***Crystals and the Solid State***
   a. Students will understand the fundamental properties of solid state, including molecular packing and the nature of bonding in molecular, ionic, and extended solids.
6. ***Symmetry***
   a. Students should be able to identify symmetry elements and nomenclature of molecular point groups and differentiate chiral and achiral species, as well as demonstrate a basic understanding of translational symmetry.
7. ***Molecular Concepts***
   a. Students will understand molecular geometry (static and dynamic) and its interpretation in terms of chemical bonding models at multiple levels of theoretical sophistication. (In general chemistry, this is an important topic and one where crystallographic results may be easily incorporated.)
8. ***Data Usage and Model Evaluation***
   a. Students should understand the nature, extent, and origins of experimental uncertainties in crystallographically derived results.
   b. Students will understand the connection between experimental structural data and theoretical models.
   c. Students should be familiar with crystallographic databases.
   d. Students should be able to interconvert text formulae, line drawings, and 3D representations.

Pre-High School K-8

> *"Friedrich Fröbel, a nineteenth century educator trained as a crystallographer, invented kindergarten. Fröbel's background in crystallography infused every aspect of his conception of kindergarten, especially the self-actuated learning devices or 'gifts' that were the centerpiece of his curriculum."*
>
> ***- B. Kahr***
> *Crystal Growth and Design, 4 (2004) 3-9*

Crystallography 'awareness' should begin in K-8 education. Students are easily enthused or put off by subjects in pre-high school, often making life-altering decisions about future study and career goals. Natural curiosity and excitement about the scientific world must be encouraged and cultivated. Crystallography, which derives molecular structure and its implications in such fields as drug discovery and materials design is a highly interdisciplinary and visually stimulating science, capable of providing cues for discussions of symmetry, chemical structure, biochemical processes and molecular disease.

Friedrich Fröbel, a crystallographer and the inventor of kindergarten, believed that the geometrically shaped surface planes of crystals demonstrated that fixed laws govern the natural world. Fröbel believed that these same laws guide the development of the child, the adult, and even whole societies, and therefore that the logic of creation could be illumined through the guided manipulation of forms. In grades K-8, National Science Education Content Standards expect science curricula to develop students' understanding and abilities aligned with the concepts and processes associated with a) systems, order and organization; b) evidence, models and explanation; c) form and function. Teachers should be given opportunities for continuing education in crystallography to give them knowledge and provide them with learning units, tools and modern examples to incorporate into their curricula, so that they are comfortable teaching science. Completion of such professional development and innovative application of the knowledge gained should be rewarded through certification and in-service credit.

Recommendations for Pre-High School K-8 Education

1. ***Models*** are tentative schemes or structures that correspond to real objects, events, or classes of events, and that have exploratory power. Crystallography is easily introduced in grades K-8 as one of the pre-eminent experimental methods for determining molecular structure. Models can be explored by students to help explain how molecules work.

2. Students' understandings about ***scientific inquiry*** can be developed through exploration of molecular structure models derived from crystallographic experiments.

3. ***Properties of materials*** can be explained through the use of crystal structures (For example, properties of the solid state of matter can be explained using household and common materials, such as table salt, ice, or snow.

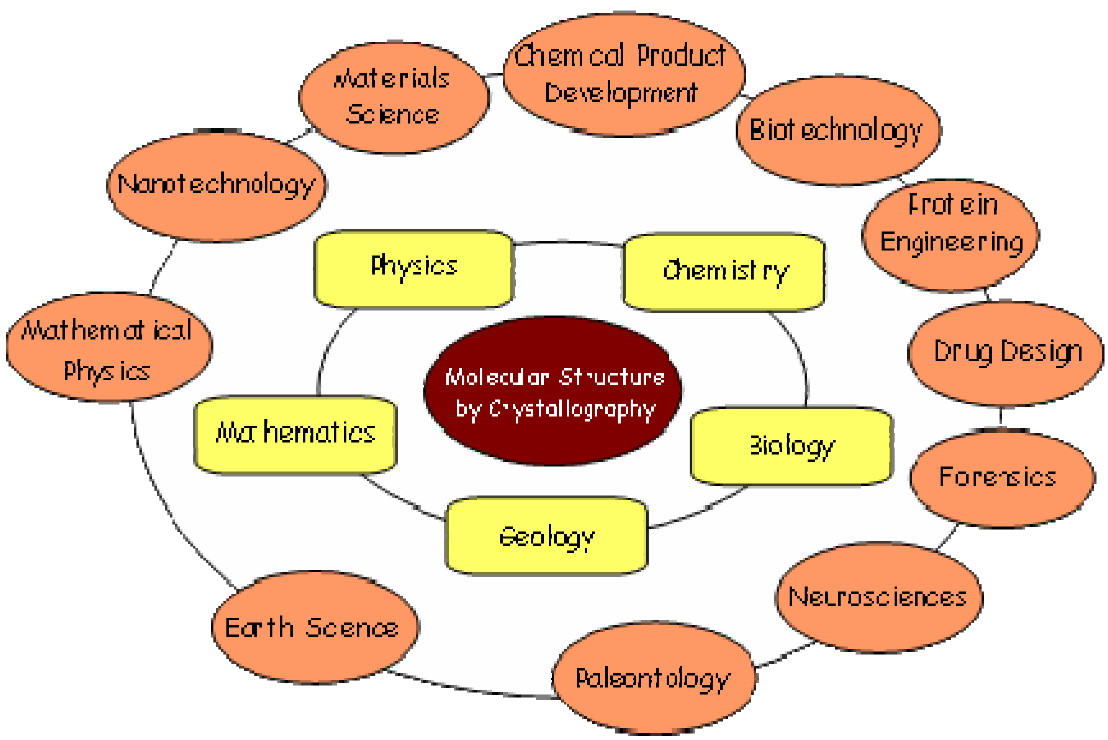
4. Students' understanding of the ***structure and function of living systems*** can be developed through the use of crystal structures.

5. Students' understanding of ***science as a human endeavor*** can be developed through discussions about crystallography, which is a highly interdisciplinary science with a fairly recent, yet rich, history.

6. The ***abilities of technology design*** may be illustrated by crystallography.

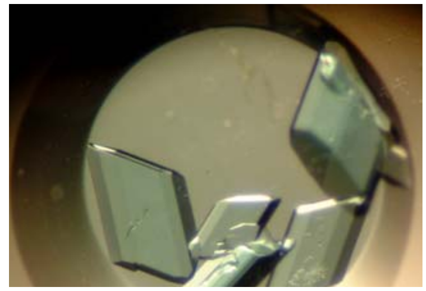
7. Students' understanding of ***science and technology*** may be developed through discussions about crystallography.

8. The ***social impact of science on society*** may be demonstrated through discussions about the biomedical applications, such as therapeutic drug discovery, derived from crystal structures.



Crystallography is a highly interdisciplinary science, bordering on and integrating naturally with fields such as earth science, physics, chemistry, biology, biotechnology and mathematics.

High School 9-12



Crystals of copper (II) sulfate pentahydrate, grown under mineral oil from a saturated solution.

High school is a significant period in the education of students, because this is when they are exposed to science at a more significant level, and when they make their preliminary career choices. Well-qualified teachers must be able to present contemporary scientific topics in a way that attracts talented and enthusiastic young people to science, whether contributing to the development of scientifically literate citizens or science specialists in the future work force. Teachers should be given opportunities for continuing education in crystallography, to provide them with knowledge, learning units, tools and modern examples to incorporate into their curricula, and to help them to be comfortable teaching science. Completion of such professional development and innovative application of the knowledge gained should be rewarded through certification and in-service credit. In grades 9-12, National Science Education Content Standards expect science curricula to develop students understanding and abilities aligned with the concepts and processes associated with a) systems, order and organization; b) evidence, models and explanation; c) form and function. All junior and senior level chemistry classes include substantial content on ionic and molecular structure, and chemical bonding, which can be elucidated within the context of crystallography.

Recommendations for High School 9-12 Education

1. ***Models*** are tentative schemes or structures that correspond to real objects, events, or classes of events, and that have exploratory power. Crystallography is easily introduced in grades 9-12 as one of the pre-eminent experimental methods for determining molecular structural models that can be explored by students to help explain how molecules work.

2. Students' understandings about ***scientific inquiry*** can be developed through exploration of molecular structure models derived from crystallographic experiments.

3. ***Properties of materials*** can be explained through the use of crystal structures. (Crystals and crystal growth can be used as an example of illustrating order and organization.)

4. Students' understanding of the ***structure and function of living systems*** can be developed through the use of crystal structures.

5. Students' understanding of ***science as a human endeavor*** can be developed through discussions about crystallography, which is a highly interdisciplinary science with a fairly recent yet rich history.

6. The ***abilities of technology design*** may be illustrated by crystallography.

7. Students' understanding of ***science and technology*** may be developed through discussions about crystallography.

8. The ***social impact of science on society*** may be demonstrated through discussions about the biomedical applications derived from crystal structures.

9. The results of protein crystallographic analysis may be used to develop students understanding of the ***molecular basis of heredity and biological evolution***, as well as ***matter, energy and organization of living systems***.

Appendix A: Biographical Information on the Summit Participants

Katherine Kantardjieff, who organized this summit, did her graduate and post-doctoral work at UCLA with David Eisenberg. She is Professor of Chemistry and Biochemistry at California State University Fullerton, a PUI, where she also directs the W.M. Keck Foundation Center for Molecular Structure (CMolS). CMolS is a comprehensive core facility for structure determination and analysis which serves the 23 campuses of the CSU, the largest public university system in the US. Her research interests are in protein structure/function with applications in bioinformatics, protein engineering and structure-guided drug discovery. Her laboratory also develops experiments in X-ray diffraction for the undergraduate laboratory which investigate small molecule and macromolecular systems. Dr. Kantardjieff has been a member of the USNC/Cr, where she chaired the Education Subcommittee from 2001-2005, and she is currently the Vice-Chair. She is a member consultant to the IUCr Commission on Crystallographic Teaching, the ACA Continuing Education Committee, and the editorial board of the Journal of Chemical Crystallography, and she is Co-Editor of the Journal of Applied Crystallography. Dr. Kantardjieff is funded by the NSF-CCLI program to host professional development workshops for PUI faculty through the Center for Workshops in Chemical Sciences consortium. In 2003, Dr. Kantardjieff was the recipient of the College of Natural Sciences and Mathematics Outstanding Teaching Award, and she has been honored four times by CSUF for her Scholarly and Creative Activity.

Elaine McClanahan served as facilitator for this summit. McClanahan received her BS in Biology from the State University of New York, and her MS in Biology from California State University Fullerton. She also holds a California Community College Supervisor Credential. She has been Professor and Chair of Biology at Crafton Hills College, Yucaipa, CA, as well as Director of the Institute for Training and Development, San Bernardino Community College District (CA). In her present positions as President, Strategic Learning, and Managing Partner, PACT Publishing and Consulting, Chino Hills, CA, McClanahan conducts interactive workshops that assist participants in the development of courses and assessment instruments in education, provides management assistance for implementation of educational grants, and plans and facilitates senior level management retreats, conferences and workshops for governmental agencies.

Jerry Bell is Senior Scientist, since 1999, in the Education Division of the American Chemical Society. He taught at the University of California-Riverside for five years and for 25 years at Simmons College, before joining the American Association for the Advancement of Science as Director for Science, Mathematics, and Technology Education Programs in the Education and Human Resources Directorate in 1992. During 1984-86 he served as Director of the Division of Teacher Preparation and Enhancement in the Directorate for Science and Engineering Education at the National Science Foundation. His major professional interests have focused on science (chemical) education at all levels, especially the use of hands-on approaches to teaching and learning. He developed and published new laboratory materials for almost all the courses he taught, is an advocate for small scale techniques in all instructional chemical laboratories, and committed to the use of lecture experiments as an effective method for communicating chemistry. In his present position, he is Chief Editor for the ACS textbook, Chemistry, and directs the Office of Graduate Education.

Robert Bau is Professor of Chemistry at the University of Southern California. His main research involves neutron diffraction studies of metal hydride complexes, especially H atoms in metal clusters. More recently, his research group has been engaged in neutron diffraction studies of proteins from hyperthermophiles to better understand their unusual thermostability. Dr. Bau has also garnered two awards for Excellence in Teaching from USC. He is currently involved in the design and building of a single crystal diffractometer at the new high-intensity Spallation Neutron Source (SNS) at Oakridge National Laboratory in Tennessee, and he is President of the ACA Council.

Simon Billinge is Associate Professor in the Department of Physics and Astronomy at Michigan State University, where he is also a member of the Quantitative Biology and Modeling Initiative. Dr. Billinge's research employs novel X-ray and neutron scattering techniques and advanced sources and modeling to study the local structure of complex materials, which range from semiconductor alloys to proteins. His laboratory also looks beyond crystal structure to examine defects and local structures of materials that are not crystalline. Dr. Billinge, who has several articles and primers on the pair distribution function method and the structure of complex materials, is currently a member of the Continuing Education Committee of the ACA.

Gloria Borgstahl is Associate Professor at the Eppley Institute for Research in Cancer and Allied Diseases at the University of Nebraska Medical Center. She has been primarily interested in studying the macromolecules essential to the maintenance and replication of DNA. Current targets include Replication Protein A (RPA) and Rad52. RPA is a single-stranded DNA binding protein that is a key player in general DNA metabolism. Rad52 was first recognized for its importance in yeast survival when treated with ionizing radiation. Rad52 forms a ring structure, binds to DNA double-strand breaks and interacts with RPA and Rad51. Familial breast cancer genes, BRCA1 and BRCA2 are also involved in this double strand break repair pathway. Dr. Borgstahl is also interested in developing methods for the quantitative comparison of crystal quality. One experimental method involves using highly-parallel, highly monochromatic synchrotron radiation, super-fine phi slicing and a CCD area detector to simultaneously measure mosaicity and diffraction resolution from hundreds of reflections at a time. Her group has written a graphical user interface program for the data processing called BEAM-ish. Dr. Borgstahl was recently elected to the Continuing Education Committee of the ACA.

Charles Campana is Senior Applications Scientist for single-crystal X-ray diffraction product lines at Bruker AXS in Madison, Wisconsin. He has extensive experience in sample analyses, P4 and SMART systems, training courses and seminars, and basic research in chemical crystallography. Campana is also Visiting Scientist in the Department of Chemistry at the University of Wisconsin Madison. He received his PhD in 1975 from the University of Wisconsin Madison in Inorganic Chemistry, working with Larry Dahl. His dissertation was entitled “Experimental and Theoretical Investigations of Dimeric and Tetrameric Metal Cluster Systems”. Prior to joining Bruker (then Nicolet) in 1980, Campana held a post-doctoral fellowship at the University of Alberta, Canada, and he was professor in the Department of Chemistry at the University of New Mexico, Albuquerque.

Jon Clardy is Professor of Biological Chemistry and Molecular Pharmacology at Harvard Medical School. His research involves what is now called chemical biology. Starting from an interest in natural products, his group is trying to answer questions involving chemical ecology, biosynthesis, mechanism of action, structural biology, and structure-based drug design. Prior to joining Harvard Medical School, Dr. Clardy was Horace White Professor of Chemistry and Chemical Biology at Cornell University, where he was the recipient of the Clark Distinguished Teaching Award. At Cornell, Dr. Clardy also served as Associate Dean for the College of Arts and Sciences. Dr. Clardy, who is a fellow of the AAAS, is the immediate past Chair of the USNC/Cr and a past president of the American Society of Pharmacognosy.

Frank Fronczek is a Research Associate and the director of the X-ray Crystallography Facility in the Department of Chemistry, Louisiana State University since 1980. An unabashed small-molecule service crystallographer, his interests are structure of macrocycles and their complexes, natural products, absolute structure, pseudosymmetry problems, and crystallographic education. He is regularly involved in teaching a hands-on graduate course in crystallography. Education: PhD in chemistry, Caltech 1975 (with Bill Schaefer and Dick Marsh); postdoctoral at UC Berkeley (with Ken Raymond), 1975-6. He is a coeditor of Acta Cryst. C, 1996-2005. Dr. Fronczek is concerned about maintaining high quality in the service environment in the face of increasing schedule pressures, the role of cryogenics in maintenance of quality, and in the future of education of service crystallographers. Dr. Fronczek is a member of the USNC/Cr and its Education Subcommittee.

Andy Howard is Associate Professor of Biology at Illinois Institute of Technology. He is also a faculty member at the Center for Synchrotron Radiation Research and Instrumentation at IIT and Chief Scientific Officer in Industrial Macromolecular Crystallography at the APS, Argonne National Laboratory. Dr. Howard's research specializations are in software for crystallographic data processing, applications of synchrotron radiation to macromolecular crystallography, development of novel protein purification techniques, and he is Co-PI on an NIH-funded Program Project in structural genomics. Dr. Howard also directs the ACA summer school in macromolecular crystallography at the APS.

Allen Hunter was trained as an organometallic chemist doing BS, PhD, and postdoctoral research at the University of British Columbia and the Australian National University. In his second postdoc and first faculty position at the University of Alberta, he began to develop his skills with single crystal diffraction. After he moved to Youngstown State University in 1992, along with his organometallic nanomaterials research, Hunter, along with Dr. Tim Wagner and collaborators at other PUIs, established the YSU-PUI Undergraduate Diffraction Consortium which. Along with Kantardjieff and other predominantly undergraduate institution faculty, Hunter founded and directs the STaR-BURSTT CyberDiffraction Consortium, a national network of faculty with teaching and research interests in crystallography supported by remotely accessible diffraction facilities at five institutions (http://www.as.ysu.edu/~adhunter/STaRBURSTT/). Dr. Hunter is most well known amongst crystallographers for his work on the teaching of crystallography at the MS, undergraduate, and pre-college levels (e.g., *J. Chem. Educ.*, **1998**, *75*, 1297-1299), and for developing models and infrastructure for remotely accessing advanced instrumentation (e.g., *J. Chem. Educ.*, **2005**, *82,* 1555-1557). In the future, he hopes to continue his efforts to build a reputation for carrying out reliable small molecule structure determinations up to and including charge density studies, for making advanced instruments remotely accessible to students in a routine fashion, and for pushing the boundaries of crystallographic education.

Frances Jurnak is Professor in the Department of Physiology and Biophysics at the University of California Irvine. Prior to joining the faculty at UCI in 1991, Dr. Jurnak was Professor in the Department of Biochemistry at the University of California Riverside. Research in the Jurnak lab focuses on the structural determination of proteins by the method of macromolecular crystallography and other biochemical tools. Biological systems currently under investigation include elongation factor Tu complexes, plant virulence factors and cancer-relevant proteins. In collaboration with UCI engineers, Dr. Jurnak's laboratory is also engaged in the development of novel technologies that will miniaturize and expedite molecular biological methods to produce soluble proteins for biochemical and biophysical characterization. Dr. Jurnak is a past President of the ACA.

James Kaduk is director of the diffraction laboratory at Innovene USA LLC. From 1985-2005, he directed the diffraction laboratory at BP Amoco's Naperville (IL) Complex, after spending 8 years of catalyst R&D. He has used the Rietveld method to characterize an enormous variety of materials encountered in the petroleum and petrochemical industries, using laboratory and synchrotron X-ray data, as well as neutron data. Dr. Kaduk is well-known for his work in ab initio structure solution using powder data. Most of his more than 70 publications deal with applications of Rietveld refinement to practical systems, including corrosion deposits, small organic molecules, coordination complexes, zeolites, and polymers. He is a Visiting Lecturer at North Central College in Naperville and gives crystallography workshops around the world. Dr. Kaduk is Chairman of the Board of Directors of the International Centre for Diffraction Data, and he is Chair of the USNC/Cr.

Margaret Kastner received her PhD in Inorganic Chemistry from Notre Dame working with Robert Scheidt. She did post-doctoral work with Michael Clarke at Boston College. Now a Professor of Chemistry at Bucknell University, she does small-molecule crystallography, primarily on transition metal complexes. She, together with several students, has written a suite of computer-based instructional units she uses with both undergraduate and graduate students in either independent study or the class room. These programs and their use in teaching crystallography are described in "Crystallographic CourseWare" (*J. Appl. Crystallogr*. **1999**, 32(2), 327-331). The programs themselves are published by J. Chem. Ed. Software, abstracted as "Point Group I, II, and III", (J. Chem. Educ. **2000,** 77, 1246) and "Crystallographic CourseWare", (J. Chem. Educ. **2000,** 77, 1247). Dr. Kastner is a past member of both the ACA Continuing Education Committee and the IUCr Commission on Crystallographic Teaching.

Cheryl Klein Stevens holds the Margaret K. Wiley Professorship in Chemistry at Xavier University in Louisiana. Dr. Stevens' research focuses on the use of X-ray crystallographic techniques for determination of the structures and charge densities of small pharmacologically interesting molecules. These molecules are dopamine agonists (used to treat Parkinson's disease), dopamine antagonists (used to treat psychosis and depression), and dopamine uptake inhibitors (used to understand cocaine addiction). Most recently, Dr. Stevens' research group has been using molecular modeling techniques to understand the relationship between the three-dimensional structures of these molecules and their pharmacological activities. Dr. Steven's also serves as the Program Director for the NIH-MBRS program at Xavier. She is beginning her second term on the USNC/Cr, where she is a member of the Education Subcommittee.

Marilyn M. Olmstead is a Professor in the Department of Chemistry at the University of California, Davis. Prior to 2003 she was the departmental crystallographer and responsible for the small molecule X-ray facility. In this capacity she has worked with many students who wished to be educated in X-ray structure determination. She serves as Co-Editor, Acta Crystallographica, Section E (2001 to present), on the Board of Editors for Inorganic Chemistry and the Journal of Coordination Chemistry, and is chair of the Continuing Education Committee of the ACA (2005). She has been a practicing small molecule crystallographer for 30 years. More generally, she wishes to support the efforts of the USNC/Cr and ACA to further fundamental education in crystallography.

James Pflugrath is Senior Applications Scientist at Rigaku/Molecular Structure Corporation, The Woodlands, Texas and Faculty in Structural and Computational Biology and Molecular Biophysics at the Baylor College of Medicine. Dr. Pflugrath's research, conducted in an industrial setting, is concentrated on the advancement of X-ray diffraction technology so that the phase problem can be easily solved and new structures readily determined. To this end, his group works in 4 main areas: data collection and processing software, X-ray sources, X-ray detectors, and robotic sample handling. They also test new X-ray sources and detectors before their introduction to the market. Finally, they are continuing to develop a robot that transfers crystals from a dewar of liquid nitrogen into a cryogenic nitrogen gas stream, automatically aligns and screens the crystals, collects diffraction images, then processes them. Dr. Pflugrath has been a regular instructor at the annual Cold Spring Harbor Laboratory course in X-ray Methods in Structural Biology, the European Crystallographic Computing School, and the ACA Summer School in Crystallography.

Kent Ratajeski recently joined the faculty at the University of West Georgia as Assistant Professor. Previously, he was an associate research professor at Montana State University. His academic interests include the igneous petrology of granitic rocks (particularly those in Yosemite National Park) and geoscience education. As part of a one-year post-doc at MSU, Dr. Ratajeski worked with Dr. David Mogk and the Science Education Resource Center (SERC) at Carleton College on a variety of projects funded by the Digital Library of Earth System Education (DLESE). One of these projects is a web-based module titled "Teaching Mineralogy with Crystal Structure Databases and Visualization Software" (http://serc.carleton.edu/research_education/crystallography) which explores creative ways to use online crystallographic data and computer graphics to promote active-learning in undergraduate mineralogy courses. .

Miriam Rossi received her PhD at The Johns Hopkins University with Thomas J. Kistenmacher. After, she went to Jenny Glusker's laboratory at the Fox Chase Cancer Center and then to Vassar College, where she is the Mary Langdon Sague Chair of Chemistry. She teaches courses at all levels of the curriculum for science majors and non-majors. She incorporates crystallographic principles and results into her lectures at any opportunity. She has an active undergraduate research program in small molecule crystallography and several of her former students have gone on to become practicing crystallographers., Dr. Rossi was recently elected to the USNC/Cr and serves on the Education Subcommittee.

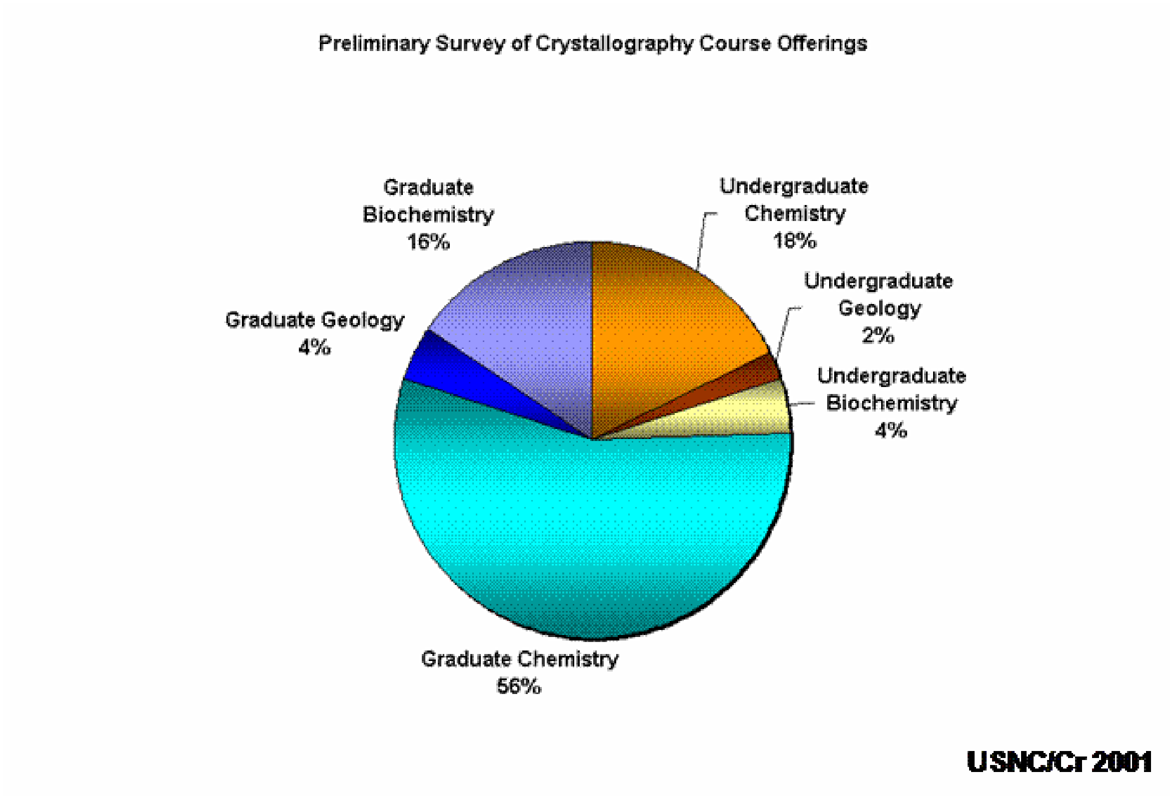
Bernhard Rupp established the Macromolecular Crystallography and Structural Genomics group of the Lawrence Livermore National Laboratory, University of California, Livermore, CA. In post doctoral and research scientist positions in the USA, Israel and Europe he has acquired a broad background in physics, material science, chemistry, high throughput protein crystallography, technology development, structure guided drug design, and structural bioinformatics. As adjunct Professor for Molecular Structural Biology at the University of Vienna, Austria, he has lectured in physical chemistry, mathematics, and structural chemistry, and now offers biennial courses in advanced biomolecular crystallography in Vienna and at Texas A&M University. In addition to classroom teaching, he developed a web-based tutorial, "Crystallography 101" (http://ruppweb.dyndns.org), which has been visited by over 500,000 students and scientists. Dr. Rupp's tutorial is used in NSF sponsored crystallography workshops and his lectures at the EMBL PEPC courses. Dr. Rupp has also organized several crystallization and structure validation workshops across Europe and the US.

Robert Sweet is the Principal Investigator of the Macromolecular Crystallography Research Resource (PXRR), which provides facilities and support at the National Synchrotron Light Source for the benefit of outside and in-house investigators. The PXRR is supported by the NIH's National Center for Research Resources and the DOE Office of Biological and Environmental Research in its mission to create optimal facilities and environments for macromolecular structure determination by synchrotron X-ray diffraction. With a staff of about 25, the PXRR innovates new access modes such as FedEx crystallography, builds new facilities, currently on the X29 undulator, advances automation, develops remote participation software, collaborates with outside groups, teaches novice users, and supports visiting investigators with 7day, 20 hours staff coverage. Along with Denise Krantz, Dr. Sweet organizes and hosts the annual Rapidata course, a practical course in macromolecular X-ray diffraction measurement providing students with an introduction to the best people, newest equipment, and latest techniques in a hands-on environment.

Iris Torriani is a Professor at the Instituto de Fisica Gleb Wataghin, Universidade Estadual de Campinas, Sao Paulo, Brazil and a staff scientist at the Brazilian Synchrotron Laboratory (LNLS). She is a member of the Executive Committee of the IUCr, and the IUCr representative to the ACA Council. Dr. Torriani is the president of the Brazilian Crystallographic Association and for more than 20 years has been teaching crystallography and solid state courses for university Physics students at the graduate and undergraduate levels. At present, Dr. Torriani's research involves studies on the folding and stability of peptides and proteins including amyloids, using small angle X-ray scattering and low resolution molecular modeling. She is also involved in the development of instrumentation for SAXS-WAXS experiments at the LNLS, where she coordinates two beamlines dedicated to biology and materials science applications.

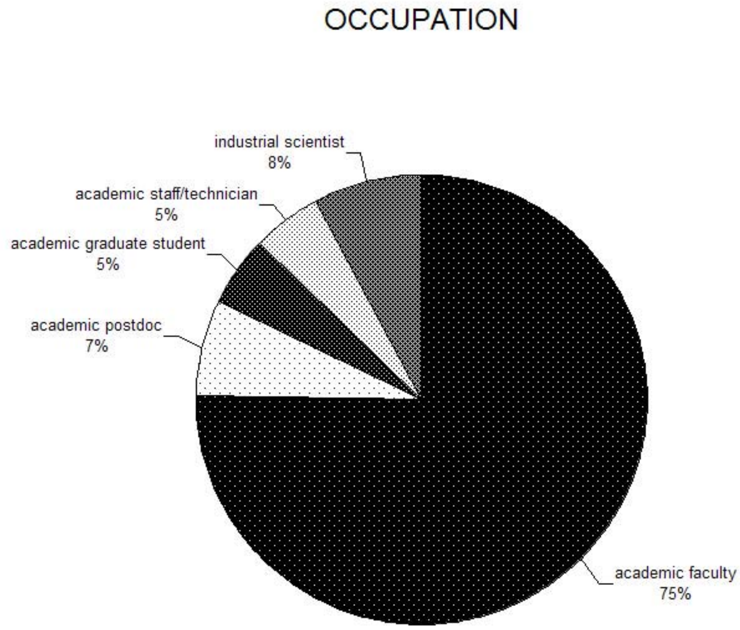
Victor Young is director of the X-ray Facility in the Department of Chemistry at the University of Minnosota, a position he has held for more than 10 years. Prior to this he held a similar position at Iowa State University for 5 years. Dr. Young specializes in twinned structural refinements. He has a strong collaboration with ChemMatCARS at Advanced Photon Source at Argonne National Laboratory with the microcrystallography beamline project, and he is part of the Spallation Neutron Source Single Crystal Diffractometer instrument development team (TOPAZ) at Oak Ridge National Laboratory. For the past 7 years, he has been actively engaged in developing courses and laboratory activities to formally train chemists in crystallography, exploiting readily available CCD technology.

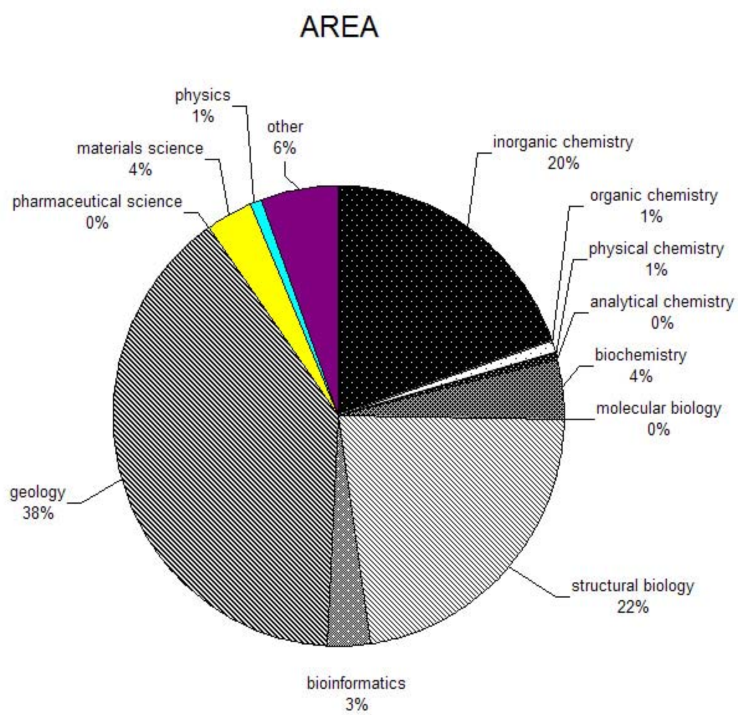
Appendix B Results of Surveys Conducted by the United States National Committee for Crystallography



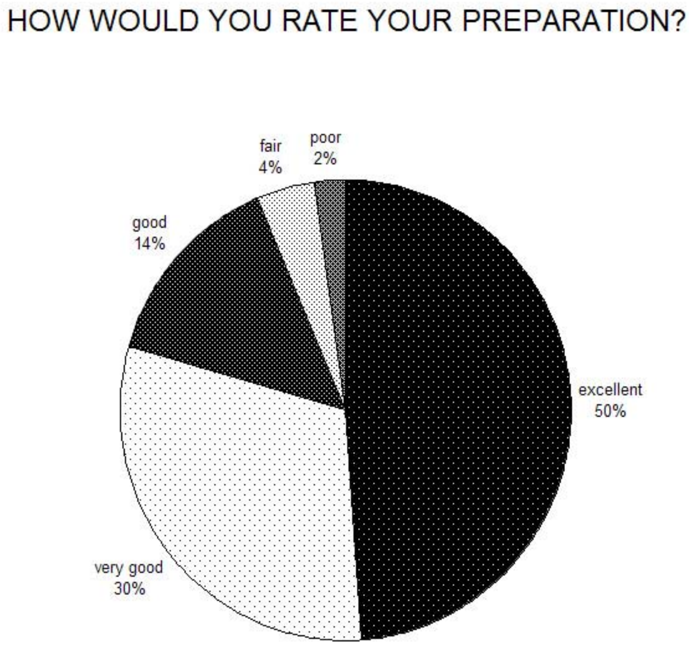
Crystallography in a College/University Curriculum

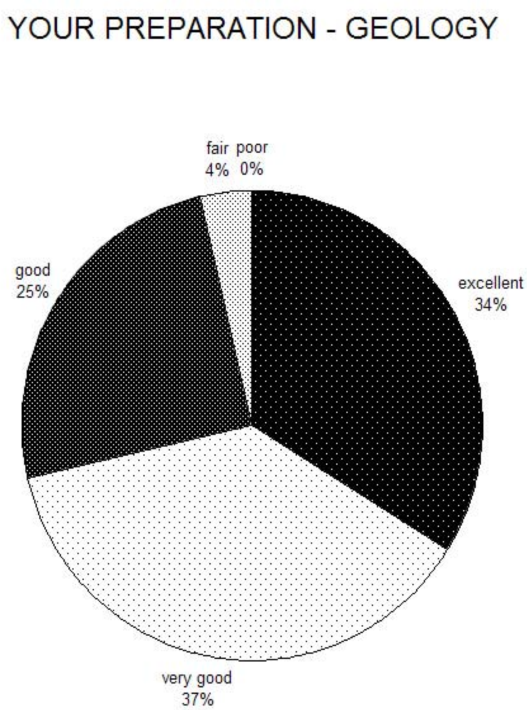
These are the results of a web-based survey prepared by the Education Committee of the US National Committee for Crystallography, given between April 25 and May 16, 2003. We asked the crystallographic community, through several popular list-serves, their opinions and views about the role and coverage that crystallography should have in an undergraduate or graduate curriculum in various scientific disciplines. There were 141 respondents with the following characteristics:



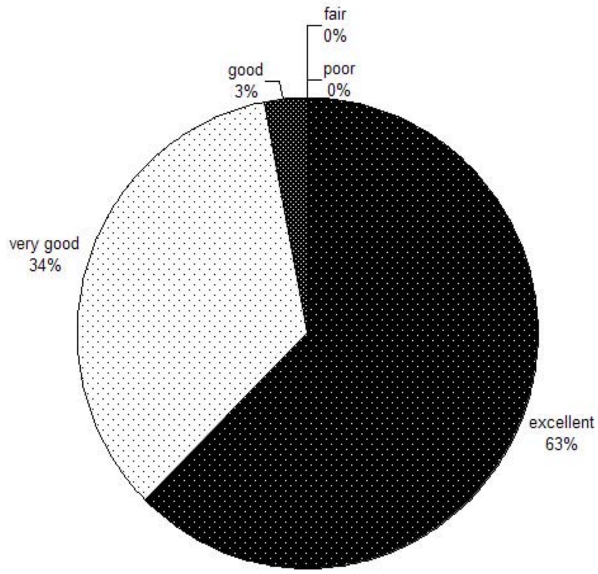


The respondents were asked to rate their own preparation to conduct crystallographic work. This is then broken down by the three largest groups of respondents: geology, structural biology and inorganic.

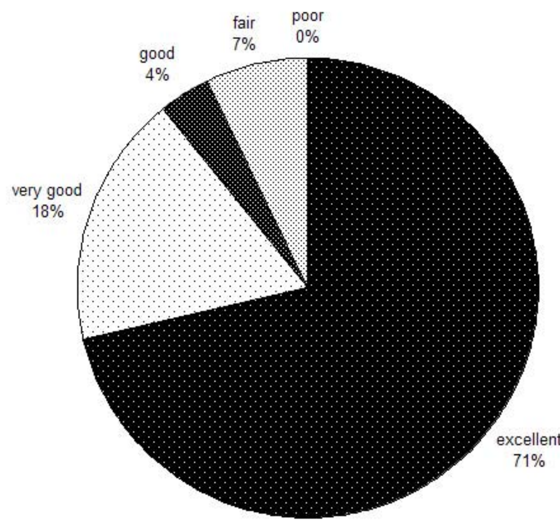




YOUR PREPARATION - STRUCTURAL BIOLOGY

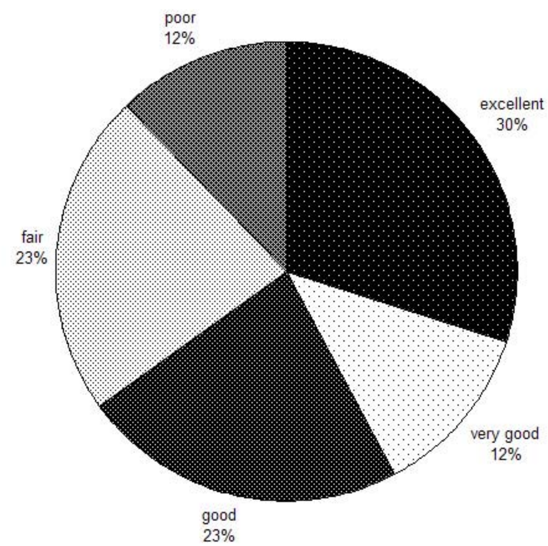


YOUR PREPARATION - INORGANIC

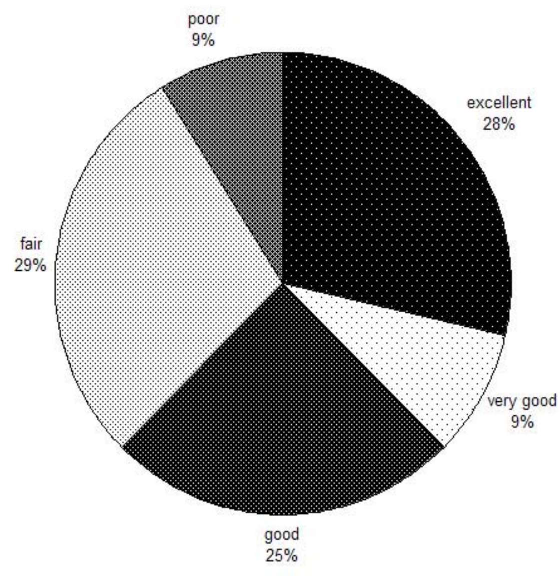


Respondents were then asked to rate the preparation of individuals that they supervise, such as graduate students, post-docs or staff-technicians. This is then broken down again by the largest groups.

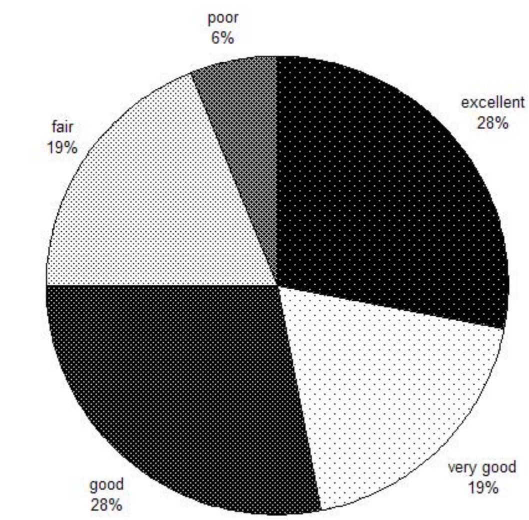
HOW WOULD YOU RATE PREPARATION OF THOSE YOU SUPERVISE?



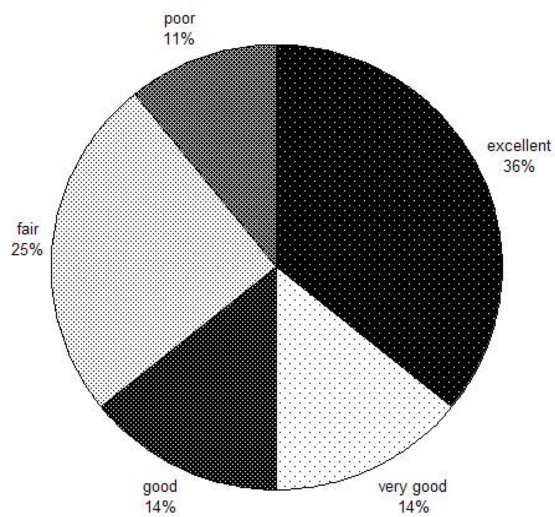
PREPARATION OF PEOPLE YOU SUPERVISE - GEOLOGY



PREPARATION OF PEOPLE YOU SUPERVISE - STRUCTURAL BIOLOGY

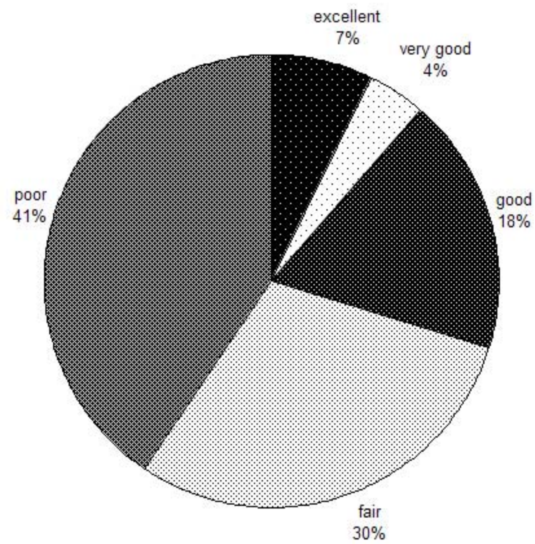


PREPARATION OF PEOPLE YOU SUPERVISE - INORGANIC

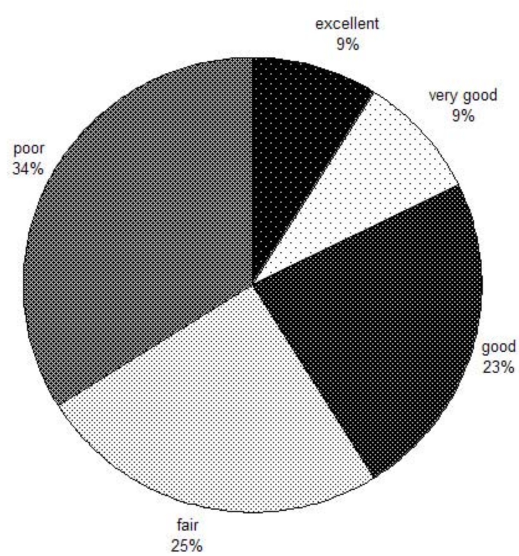


Respondents were then asked how they felt about the coverage of crystallography in the *under-graduate curriculum* overall. The responses are also broken down by the three largest groups.

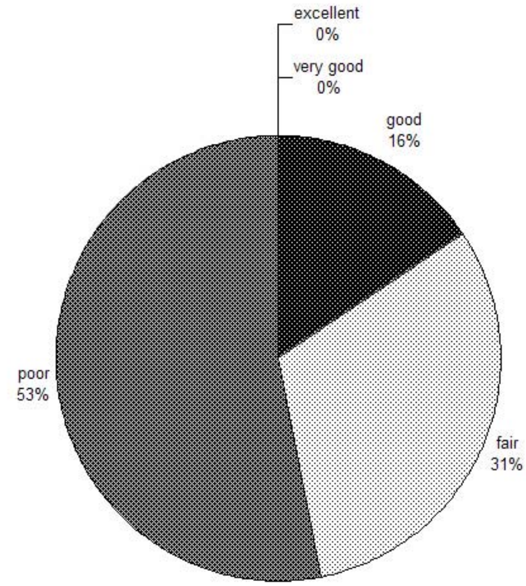
COVERAGE OF CRYSTALLOGRAPHY IN THE UNDERGRADUATE CURRICULUM



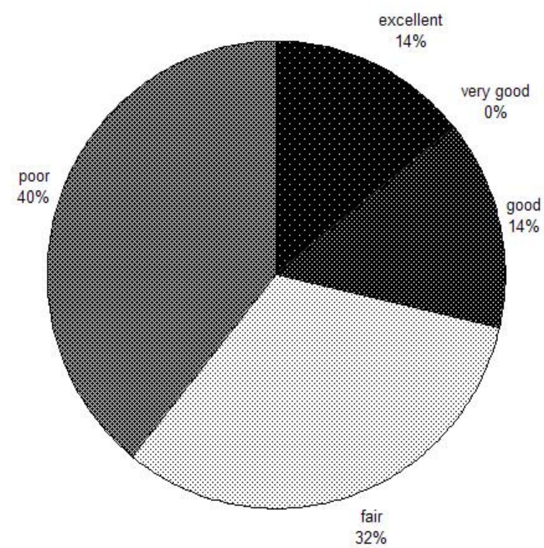
COVERAGE IN THE UNDERGRADUATE CURRICULUM - GEOLOGY



COVERAGE IN THE UNDERGRADUATE CURRICULUM - STRUCTURAL BIOLOGY

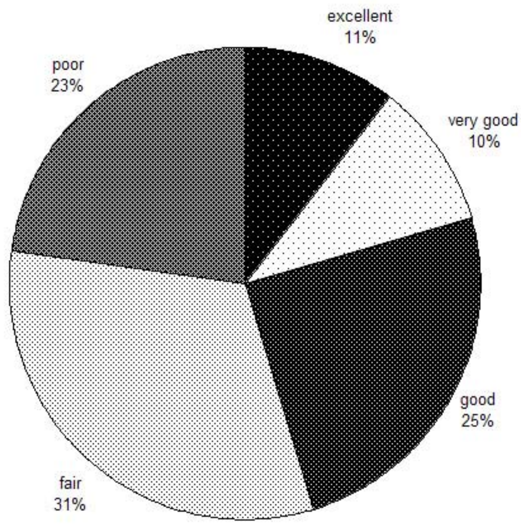


COVERAGE IN THE UNDERGRADUATE CURRICULUM - INORGANIC

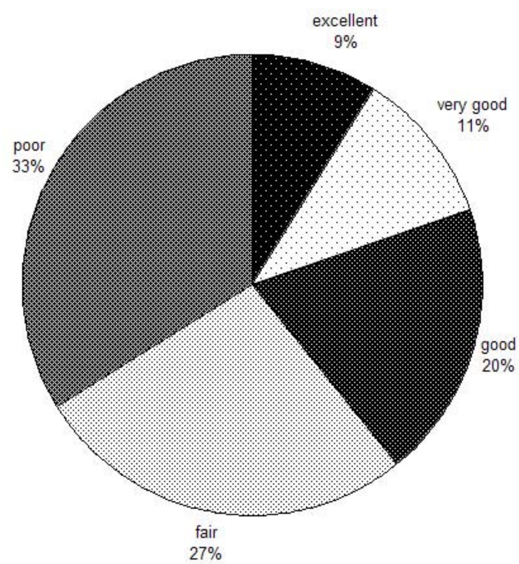


Respondents were then asked how they felt about the coverage of crystallography in the *graduate curriculum* overall. The responses are also broken down by the three largest groups.

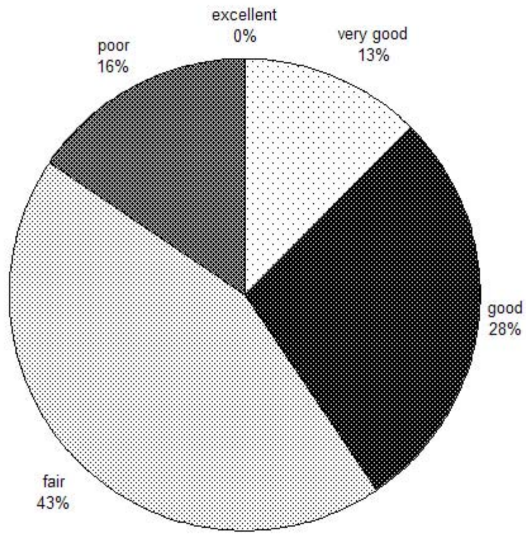
COVERAGE OF CRYSTALLOGRAPHY IN THE GRADUATE CURRICULUM



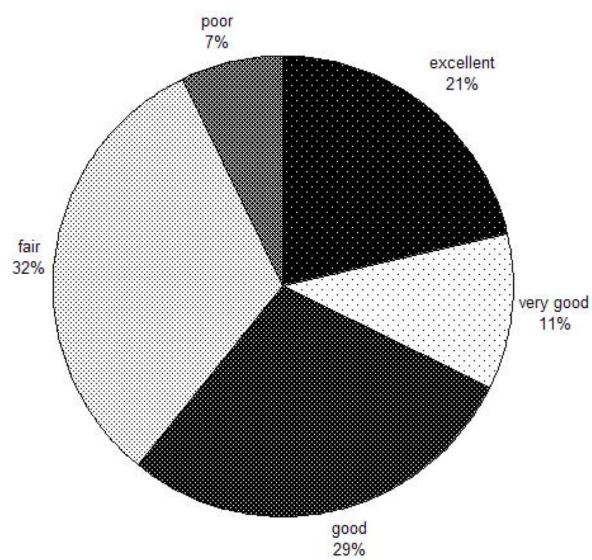
COVERAGE IN THE GRADUATE CURRICULUM - GEOLOGY



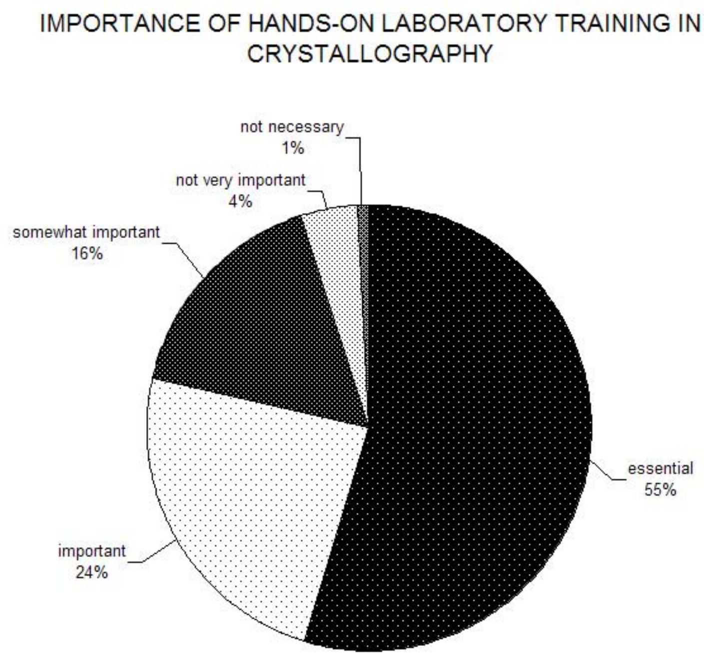
COVERAGE IN THE GRADUATE CURRICULUM - STRUCTURAL BIOLOGY

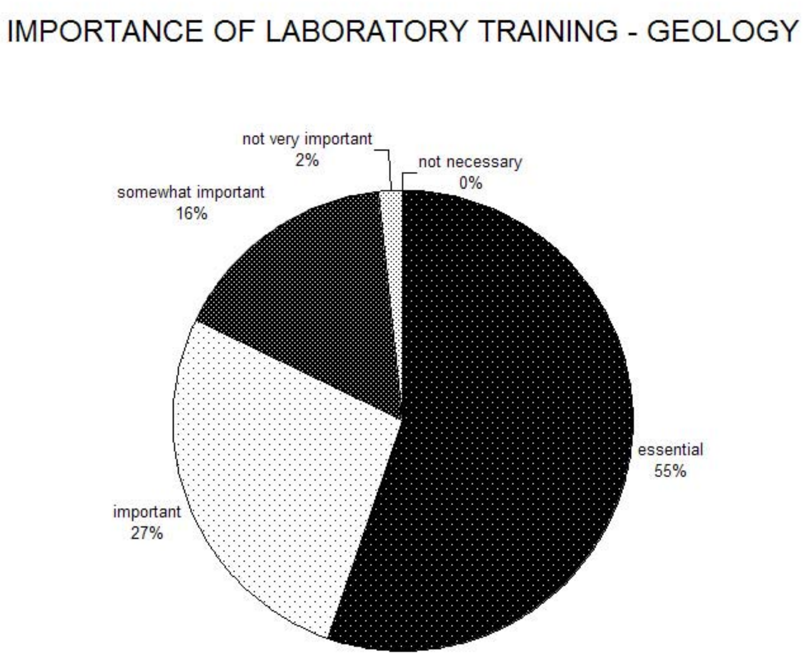


COVERAGE IN THE GRADUATE CURRICULUM - INORGANIC

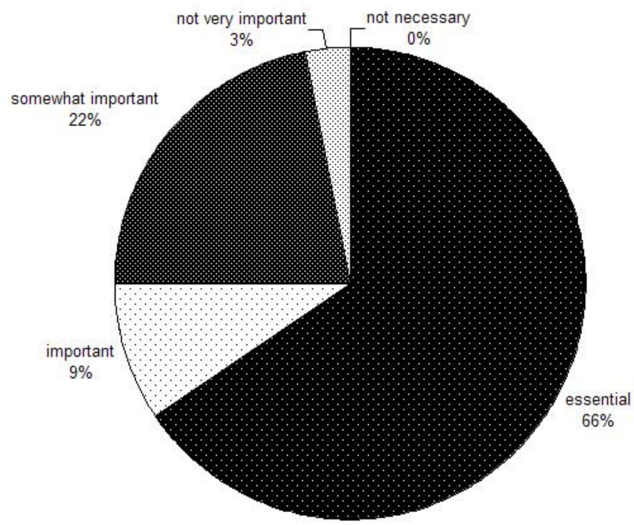


Finally, respondents were asked to comment on the importance of hands-on laboratory training in crystallography. The responses are also broken down by the three largest groups.

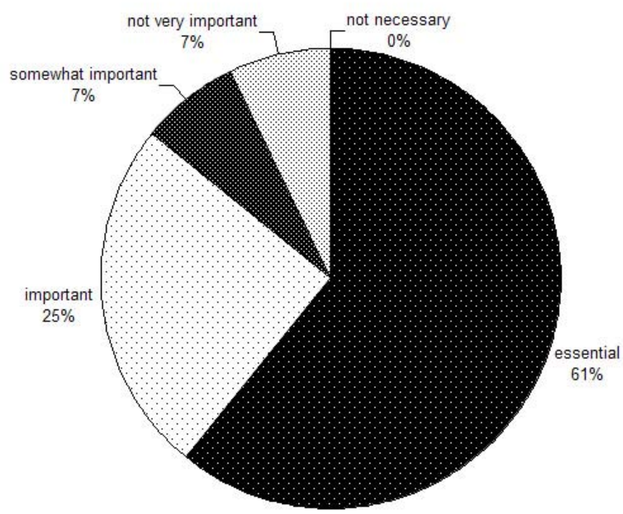




IMPORTANCE OF LABORATORY TRAINING - STRUCTURAL BIOLOGY



IMPORTANCE OF LABORATORY TRAINING - INORGANIC



Respondents were asked to make specific comments either explaining their answers to the previous questions, as well as make specific suggestions about curriculum content, coverage and the like. They were also given the opportunity to make additional comments or provide information for which we may not have specifically asked.

Regarding their own preparation, respondents said:

I have done more than 50 xtl structures per year for the last three years.
I have good theoretical crystallographic knowledge with lots of experimental experience.
Although I have solved a number of structures, I feel that I am still a novice. There are data sets that give me problems and my success rate at solving these problems is only forty to fifty percent.
Graduate school + 5 postdoc years + service crystallographer.
I trained with an expert and I have 22 years experience.
We have everything is in house, good X-ray facility, graduate students are trained and use the facility independently.
Took one year class in X-ray crystallography in graduate school taught by Jerry Donohue. Several years doing powder diffraction and then a Fulbright award to work with Mario Nardelli and Antonio Tiripicchio in Parma, Italy. Several years doing single crystal crystallography and ~two years as Director, Small Molecule X-ray lab at Caltech. Currently, Director, X-ray Crystallography Center, Emory University.
I never had any training in structure solution but was trained as a solid state spectroscopist.
I was a graduate student of a crystallographer and pursued a crystallographic postdoctoral position.
I learned from Dick Marsh.
I have been the instrument operator for a year and a half and am fairly competent that I work efficiently and produce quality results.
A course as an undergraduate. A course as a graduate student. Three sabbatical years.
As a graduate student at The University of Windsor, we had hands-on access to the Rigaku AFC6 after taking Doug Stephan's course in X-ray crystallography. At The University of Western Ontario I went from my postdoc position to staff crystallographer when they needed someone to run the newly-arriving Nonius Kappa-CCD (and thanks to Nick Payne for help along the way). I also went back to Windsor to use their Siemens CCD instrument, which is what I have now at Saint Mary's University. A lot of my "preparation" has resulted in my being in the right places at the right times, and having to learn "on the fly" as it were.
Adequate teaching as a grad student 1960-63 and excellent post-docs with Gene Carpenter(Brown) and Jim Ibers (Northwestern) '64-'66. 36 years research & teaching since.
In my formal education I had very little crystallography.
I am largely self-taught. I did sit in on a crystallography course in 88.
Ph.D. in P.Chem, major emphasis in small molecule crystallography, and postdoc in small molecule crystallography, including Laue and powder diffraction work.
I don't do crystallography myself; I collaborate closely with crystallographers, and I use the results of structure determination in several areas of research and teaching. In the latter area I have developed and now teach a course in homology modeling of protein 3D structures to advanced undergraduates and graduate students. I also give a lecture on crystallography in General Biochemistry, our one year survey course, and I use struc-

tural material extensively in the course for undergraduates.
Trained on sabbatical leave in an active protein X-ray crystallography laboratory. Have personally crystallized, collected data for, and solved structures of one or more new proteins.
The only crystal structure I remember seeing from undergraduate school was that of hemoglobin.
We have all the necessary instrumentation and computation hardware available for small and macromolecular crystallography.
Trained in a great crystallography lab, taken a few classes.
I am a crystallographer who is very prepared because of experience. However, I feel that the formal teaching in crystallography I had was weak.
PhD and postdoc in crystallography.
Graduate work in a basic science (immunology) followed by post-doctoral work in an excellent crystallography laboratory has prepared me well for a career in either academics or industry. The basic science background is very important - with crystallography as a tool - and not a 100% vocation.
I trained in a lab were all aspects of a protein crystallographic problem, from construct design to refinement, were the responsibility of the researcher. I bring that broad training to my job.
Formal training in structural biology.
Solid foundation of training in small-molecule and macromolecular crystallography in a Chemistry department; began with fundamentals of diffraction and learned biology later.
First degree physics second degree physics-crystallography PhD chemistry-crystallography.
As a graduate student I was mentored in an excellent structural biology lab and have continued my research in a highly respected crystallography lab.
My undergraduate degree is in chemistry and I did my Ph.D. in a PX lab. I took a number of molecular biology courses in grad school.
I consider on the job instruction to be sufficient. A small number of hours of theoretical instruction provide a very good preparation. Crystallography is a technique, not a science.
It would have been nice to have a more comprehensive crystallography course in graduate school.
Obtaining PhD doing crystallographic research. A few valuable resources (i.e. faculty) have guided my progress. While much of the learning process has been left up to me, they provide the sources from which I learn.
While mentoring in graduate school and industrial experience gave me with an excellent appreciation of the nature of protein and nucleic acid structures and how they are created, I have not solved a structure myself and therefore feel I have much more to learn about the mechanics.
I was taught by leaders in the field. I've solved a number of small molecule structures so I know what crystallography can do. I've worked on a number of large molecules, so I know where the problems lie.
Have listened to most of the pioneers who developed the methodologies of x-ray crystal structure analysis - Bragg, Buerger, Lipson, Cochran, Belov, Ramachandran, Rossman, Perutz, Kendrew, etc
I don't do crystallography at all. I do protein-structure prediction using the models in

PDB.
I did my master and PhD in crystallography in England, but I did not have any background prior to my undergrad studies. I believe I would benefit much (very much) more of my master and PhD studies if I had prior knowledge of this area.
I had some instruction in crystallography and structural biology in undergraduate and graduate classes, and in my graduate research, but on the whole the instruction was not of very high quality, and I've probably learned more on my own than what I've been taught by others.
Not applicable. I have never done crystallography and have no plans to do any.
Graduate level courses and thesis relating to small molecule work.
I studied crystallography during my Masters, PhD, and during my post-doc. I am well-prepared.
Course work in crystallography/mineralogy, single crystal structure analysis, x-ray diffraction techniques and analysis. Used powder x-ray to identify phases, order/disorder, etc. for my M.S. and Ph.D. work.
I had undergrad and grad courses in x-ray crystallography as well as undergrad and grad mineralogy.
I am a graduate student in Mineralogy, whose thesis focuses on crystal structure determination and crystal chemistry.
I work with crystallographers who are able to help me.
I had graduate training in both powder and single-crystal X-ray diffraction, including detailed treatments of disorder.
I have had to learn much of the material myself, as formal practical courses were not available.
Basic courses in X-ray diffraction of powders and oriented clay mineral mounts
Background in powder diffraction - clay minerals, ceramics, and volcanic ash/bentonites.
I am not conducting active crystallographic research. My principle involvement is in teaching concepts of crystal structure and crystal chemistry in the context of mineralogy. My training in prior courses in mineralogy and crystal chemistry has been adequate to support the material I cover. My background is really insufficient to allow me to do contemporary kinds of crystallographic research.
I earned a PhD in geochemistry/clay mineralogy.
It would have been helpful if a crystallography course had been required somewhere along the line, perhaps grad school.
I had several weeks of crystallography as part of an undergraduate mineralogy/crystallography/optical-mineralogy/geochemistry course. What I had then was way over my head. I used XRD a lot in graduate school, and had one good course in crystal chemistry. I have taught myself quite a bit of morphological crystallography over the years, and between self-teaching and short-courses, I am comfortable with routine diffraction (e.g., XRD & HRTEM).
I have attended top ranked Universities and hold a fellowship with a preeminent laboratory.
As a petrologist, I learned enough to give me a good background for that subject and microscopic petrography and to understand what was going on in certain experimental work involving comparison dilatometry and piezobirefringence. I had rudimentary training in space groups.
PhD in crystallography.

I had courses in crystallography in graduate school.
Good training in the field as a graduate student at Michigan.
I know enough to understand powder diffraction and do my job. I feel that my mineralogy and X-ray crystallography professors did an adequate job in preparing me.
Undergraduate and graduate course work in crystallography.
Undergraduate and graduate training in 1968-76 in geology departments undergrad course in crystallography/mineralogy graduate school TA for C. Klein cryst/min course graduate course in X-ray crystallography.
I had some training in grad school but have not kept up with it.
Graduate training in mineralogy and 25+ years experience.
As an undergraduate, I was trained by a student of C. O Hutton. We learned CRYSTAL-LOGRAPHY, or as much as could be taught in 1/2 semester, not just the minimum amount required to teach systematic mineralogy.
Basic course work forms the foundation for my use of XRD, but no training was available in effects produced by disordered structures.
Undergraduate course work in crystallography in geology and metallurgy. Graduate work in crystal structure determination in chemistry.
2 years of mineralogy seem to have adequately prepared me.
I am a geologist/petrologist that deals with minerals mainly from the point of view of their chemical composition and P-T stability in igneous and metamorphic rocks. I do not do crystallography per se as part of my own or my students' research.
I had a proper education and have many years of proper experience.
B.S., M.S., Ph.D. Geology
Crystallography was my major concentration in graduate school.
My current work involves introducing undergraduate students to crystallography and mineralogy. My preparation as a student at Ohio State was far more thorough that needed to do that.
Ph.D. in crystallography from Harvard.
I have 20+ years of experience working with crystal structures of minerals, a good theoretical knowledge of X-ray crystallography, but little experience in crystal structure determination.
I've learned on-the-job most of what I teach.
Ph.D. from Virginia Tech (Mineralogy), extensive experience.
Published single crystal structure refinement by XRD.
Grad education in mineralogy.
Grad level course in crystallography and crystal chemistry (inorganic, geologic).
My undergraduate degree is in Geology, while my masters degree is in Ceramic Science. My course work has given me a "very good" preparation for crystallographic work. A mentor provides one with an "excellent" preparation. This is something I have missed.
The question is not clear to me. I feel I have a better-than-average background in crystallography and powder diffraction.
I am partially retired. My major professor was Dan McLachlan, a former president of the ACA, I also had training in neutron diffraction and worked as a postdoc with Theo Hahn's group in Aachen. I have built my own equipment and taught x-ray diffraction courses.
I know crystallography, theory and equipment, and have made significant contributions.
Excellent crystallography/x-ray diffraction class as a materials science undergraduate.

My graduate work focused on the use of HRTEM and XRD for the characterization of nanocrystalline materials. I have taken a number of courses that either focused on or included material on the crystal structure of various natural and synthetic materials - Mineralogy, Inorganic Chemistry, Solid State Physics, Ceramics, X-ray Diffraction, and Transmission Electron Microscopy.
I learned crystallography from one of the best set of educators in the world, at Cambridge University.
I got my PhD for small-molecule structures and have been doing them with various equipment for the last thirty years. My prep had better be excellent.
No formal crystallography courses -- just some basics in my intro to mineralogy in college and then self-taught.
Good formal training good experience in lab (as postdoc).
I've learned my crystallography by summer and sabbatical collaboration with structural biology labs. So I've never seen a protein project all the way through, and my preparation is spotty.
I was trained as a chemist, my Ph.D. is in chemical crystallography and my post-doctoral work was in protein crystallography.
Taught by Judith Howard, David Watkin, Jerry Atwood, Guy Orpen.

Regarding the preparation of those supervised, respondents said:

No longer any formal training.
I teach undergraduates, and there are no crystallography facilities here.
Most undergraduate courses do not teach crystallography. Therefore, most undergraduate students have no knowledge of the subject.
My co-workers are primarily trained to do synthetic chemistry and largely rely on me for their structural analyses.
Only since the advent of readily available CCD detectors has it been practical for routine use for characterization. We mostly deal with synthesis and catalysis. It is often more efficient to have a staff crystallographer do the structural analysis.
Limited to non-existing theoretical know-how, some experience with shelx.
None of the students I supervise have had any crystallographic background.
All receive several years of instruction and do 100-200 structures each.
X-ray crystallography course taught here at Emory every two years, but primarily a lecture course.
It depends on experience and their experiences differ. However, it is usually possible to find a postdoc who can do the work given additional training on the job. I do not supervise graduate students.
They all have the mathematical tools, but lack the interest in crystallography *per se.*
12 lectures on the vocabulary of the crystalline state at 3rd year and 12 on Advanced Structural Methods at 4th year plus attention in a research group with varied experience.
Only postdocs from European countries seem to have much preparation.
No full course here to teach fundamentals in diffraction; only survey courses offering a few lectures in crystal growth, data collection, phasing, and structure solution.
Very few have any crystallographic training at all. Those who do work in structural labs.
I actually supervise UNDERGRADUATE students in an active research program. They have essentially no exposure to crystallographic methods.

Lack of formal training in Crystallography hampers the research.
I have carefully explained the application of crystallography and of the underlying theory to a number of graduate students.
It depends on who it is. Many biochemistry graduate students don't come in with enough math and chemistry. Some of my postdocs don't really know how to do crystallography.
Most people do not have the foundation in mathematics, or physics, or physical chemistry that it takes to quickly learn crystallography.
The level of training obtained "on-the-job" makes them excellent researchers. Good scientists will make good crystallographers.
Many know parts they use but lack depth.
Most students have minimal if any exposure to crystallography before coming to my lab. Some postdocs have no exposure, might be trained as biochemists and some have excellent exposure. They are normally trained in the lab and with the supplement of the postgraduate CSHL crystallography course and Rapid Data collection course at NSLS. The students in the CSHL Watson School of Biological Sciences get a one week exposure to structural biology with the main goal of being able to read papers critically.
Biochemists-turned-Structural Biologists generally have poor to inadequate training and understanding of the physical concepts surrounding the science.
Mostly biologists with essential training in math, chemistry and physics.
They have or receive on-the-job training.
I've known several people who have completed PhDs in protein crystallography who have only hand-waving knowledge of crystallography. They certainly would not be able to determine structures independently.
I'm not impressed with the quantitative or computational skills of most students. They're better on the biochemistry though, which is probably a wise vocational choice.
Crystallography has become automated, one needs no knowledge of crystallography to solve structures!
Mostly, I prepare the graduate students for work in crystallography. Most grad students do not have sufficient undergraduate preparation in crystallography to do small molecule work.
They get a course in point groups, one in space groups, one in derivation of the structure factor equation. Each course is one semester.
Some have a weak background. Most do not have much.
We no longer have an analytical techniques course where training is provided.
There is virtually no presentation of quantitative information in undergraduate curricula in the geological sciences.
Little emphasis on crystallography.
Need more applied work in crystallography.
Due to equipment constraints (still using an old Phillips tube power supply, manual and modified computer operated goniometer with variable slit control for low 2theta applications), single crystal work can only be done by camera (photographic film). Peak matching software and graphics on Phillips not very good. Have to use another software package on my MAC so as to get better interpretations.
Most have even less formal training than I did, and they haven't had time to teach themselves.
Emeritus. I don't know for sure. But my observation is that they are largely ignorant of the basics even at the most elementary level even when it applies to their own work.

That also applies to incoming younger faculty, many of whom make mistakes based on their lack of understanding of symmetry in understanding petrological phenomena.
I am currently a casual user and do not stress crystallography among our research group.
The technician I work with never had training in crystallography other than what I have given him.
They have a basic understanding of symmetry elements and crystal structure.
Fair to good because many undergraduate geology majors no longer are required to take a crystallography course.
Very few of my students have ever done any powder diffraction work in classes.
I do not supervise, but those I have seen around me are generally well prepared, but some need remedial work.
Training is on a "demand" basis and is not part of formal course work.
Current curriculum does not provide students with in-depth training. Most of what they know is learned on the job or by monkey-see; monkey do. Little or no thinking or understanding of the reasons why things are done.
General departmental support for mineralogy is waning.
I have a broad spectrum of students, and this is a guess on the average.
It is difficult to find students in geology with adequate background.
Not as much time devoted to pure crystallography as in the past.
Most of my students have had a basic introduction to powder X-ray diffraction and one course in mineralogy.
Grad students come quite limited in their crystallographic background, but they learn quickly.
We don't teach crystallography at the graduate level.
Few geology programs teach crystallography at the undergrad level.
As an industrial scientist in a microscopy and X-ray diffraction group I find that many of the chemists I provide results for are poorly prepared to understand the crystallographic aspects of their work. Technicians are even more poorly prepared.
Most students I have been directly involved with do not have a strong background in crystallography.
We have up-to-date x-ray crystallographic facilities and experienced academic and technical staff.
With the exception of students who have taken a course in Mineralogy, I find it rare that students obtain an adequate preparation in crystallography. Those graduate students focusing on Mineralogy or Materials Science and/or Chemistry usually have a decent level of preparation, but I wouldn't call it very good or excellent.
Generally, those taught on our own degree programme are much better prepared than incomers.
As manager of a service lab, all students must pass an evaluation to be allowed to use the instruments. If their prep isn't at least "good", I don't have to deal with them.
My students are from life sciences. Their background in Physics and Math is not very good.
No prior hands-on.
Most of the students and post-docs who reach my group have been chemistry majors and/or Ph.D.'s and have essentially NO relevant background in this subject.

Respondents made the following comments with regard to coverage of crystal-lography in the *undergraduate curriculum*:

I teach an elective course taken simultaneously by graduate and undergraduate students. This course is designed to provide these students with a practical understanding of the use of x-ray crystallography methods for molecular structure determination.
Inorganic grad students are provided ~ 6 week discussion of crystallography and how interpret the results of published structures. Although they (the computer really) actually solve a structure, they don't have the background to successfully deal with incorrect space choices or problematic structures.
Apart from inorganic structural chemistry nothing taught.
Crystallography may or may not be covered at all. Usually the coverage is minimal and perhaps only covers a very small amount of the topic.
Proper coverage of the subject matter requires access to equipment. Thus schools with facilities tend to limit the use to graduate students, staff, and/or faculty. Hence, the coverage is fair. Also, the American Chemical Society does not consider crystallography as required topic for undergraduates.
Just a brief overview is sufficient at the undergrad level. It's too complicated to give any real understanding in a survey course.
Only about 1-2% of the undergraduate curriculum addresses the crystalline state. Most new directions in chemistry relate to the solid state. Far more coverage is needed.
Most students are just taking the class.
Very little instruction given to undergraduates in X-ray crystallography principles and techniques in most university curricula, with few exceptions.
It doesn't exist. Most of what is taught is either irrelevant or incorrect.
It is important, however covering the topic in just 1 or 2 lectures does little to promote the understanding of the subject to undergraduate students. I encourage undergraduate students to take a graduate course if they have sufficient interest in the subject.
It's barely mentioned in the freshman course or in p-chem. We offer one introductory course, but rarely are there more than two undergrads in it.
I was only briefly exposed to crystallography as an undergrad. If I had known more about it, I may have been able to start my learning process sooner.
It is mentioned in two courses, but not discussed in any detail.
I try to introduce it in my advanced inorganic chemistry course, but it's difficult to do so. We don't have room in our curriculum to add new courses because we don't have the faculty members to teach them...but my honours students on the other hand, learn a fair bit about crystallography and are at the very least, conversant.
24 lectures impart fundamentals all graduating chemists should know but do not make practitioners. Practice does and mini research projects can engender enthusiasm for more.
From word of mouth, I am not impressed.
We do little formal training and use it primarily as a turnkey structural tool in laboratory work.
Typically only lectures about NaCl and cubic closed packing, and Bragg's law. Should include more on fundamentals in symmetry and general diffraction theory.
Poor refers to the national scene. Here at Rutgers it's spotty. Some students gain some

familiarity, while many don't. There is no way for students really to grasp macromolecular crystallography until they have had a course in biochemistry, including a good dose of protein and nucleic acid structure. As they are usually 3rd year students by the time this happens, we are left with the second semester of the junior year and the two semesters of the senior year for specialized courses. It is hard to do full justice to crystallography in a one year survey; so far the best I've been able to do is give them some idea of what it entails and what one can learn from it.
Practically non-existent, other than the passing mention that all the pretty structures are determined by this method. Virtually no understanding of the methodology, the strengths and limitations of crystallography, or evaluation of structure quality, is conveyed in any standard undergraduate text that I know of. Some institutions do use molecular visualization tools to view PDB files, but these structures are usually not understood as models, but rather as actual molecular structures without uncertainty.
It depends upon the course and the instructor so much that this question, and the responses, will probably vary drastically from institution to institution. Only because there are several of us here that emphasize different aspects do I think it gets above average emphasis here.
No crystallographic teaching at this level.
They don't mention enough.
Crystallography was barely mentioned in my undergraduate studies.
I think undergrads only need a flavor of the technical details and a clear understanding of how to look at and evaluate the quality of structures.
I do not think that it should be stressed for undergrads. They have enough to work on.
I don't know the current state of crystallography coverage in undergraduate courses. When I was an undergraduate the training was hopelessly outdated compared to the state-of-the-art.
Too little and more interest in buzz words.
I rarely encounter undergrads or grad students who had previous courses in crystallography.
Much too cursory.
Very little crystallography.
Is it needed?
Students are rarely given the basic introduction to understanding how a protein structure is determined or how to evaluate the structural data. At best most students have only been taught rudimentary skills for manipulating a PDB within a graphics program.
Essentially nonexistent. The results from structural biology are covered but crystallography is not covered.
Acceptable. For those interested in molecular biochemistry, an appropriate course was available.
Consisted of a brief mention as a portion of one lecture.
Students seem to have some understanding of where structures come from but have little idea of how to appreciate them and critique them. I believe the latter should be emphasized over more technique based training at the undergraduate level.
Biochemistry majors at many schools can graduate without receiving any significant coverage of crystallography.
I'm not convinced it's something undergrads need to learn about.
Crystallography has become a tool!

It is really a postgraduate topic in biochemistry/biology.
In general not enough courses of theory are provided to have a good background. Most students do not have enough math courses to understand the math behind the computations involved.
I don't know much about what prep the undergrads get.
Crystallography in any detail is too advanced for most undergrads. Accessible and understandable visualization of macromolecular crystallographic results can be improved. RasMol and MAGE made a good start a decade ago. My Protein Explorer project is designed to help.
Not sufficient to be a crystallographer but sufficient background for most.
Not enough time to cover crystallography in sufficient detail along with all the other things that they need to be taught.
Too often crystallography in geology is skimmed over because mineralogy is combined with undergraduate petrology courses.
It is being superceded by environmental and low-T geochemistry.
Crystallography is introduced in the mineralogy courses.
It is only introduced briefly in a Mineralogy class (which I teach).
Virtually all of the graduate students with whom I work have little or no background in crystallography. For example, they know nothing about space groups, don't even know what the International Tables are, although they might know the Bragg equation.
Basically being phased out.
Given the pressures in the earth sciences to teach a very broad range of topics, crystallography has fallen far down on the list of priorities.
Very limited introduction to crystallography.
No time - that's the problem - in mineralogy can only address it with respect to crystal chemistry and crystal structure. Advanced mineralogy only offered every two (2) years and powder diffraction is a module of three (3) weeks.
I feel it is good for the undergraduates in our geology program in that it provides sufficient background for students to 1) discover whether they like crystallography and would want to pursue it in grad school, 2) is adequate to enable them, if they are interested, to collect and interpret routine powder XRD patterns, 3) use crystallographic and crystal chemical concepts predictively in thinking about petrologic processes and reactions.
The person currently teaching mineralogy (where crystallography is taught) is primarily a petrologist.
Cryst. is a forgotten area and viewed as a highly specialized area by non-mineralogists in geology. Therefore, it is not included in an essential way in the curriculum.
I have had to cut more and more out to accommodate other aspects of Mineralogy - and - we have cut the optical course entirely - which means much less coverage than I would like. The students do not end up with complete enough coverage to allow them to do research into crystallography topics. They are not confident enough of the material to be creative with it.
I can't tell whether they are taught crystallography that's too hard and they forget it because they never really learned it, or they don't cover it in class at all.
I suppose it depends on the University in question, as well as students' choices as to curriculum.
Most geology departments have reduced the preparation in crystallography to make room for environmental geology topics.

We have new faculty in this area, and I just do not know yet. Our previous faculty member, recently retired, was Buerger-trained and top-notch in assisting those of us with less sophisticated backgrounds in crystallography as it relate to petrological problems.
Varies greatly from institution to institution!
It is well presented in my Mineralogy text (Klein) without going into too much detail for a "typical" mineralogy course.
In my mineralogy course, I do not have much time to spend on crystallography.
I teach enough crystallography for geology students to appreciate the topic and use if to help them in their work. However, there is not enough crystallography in the curriculum for them to put it to research use.
We have converted traditional Mineralogy credits in our undergrad curriculum to breadth in the expanding fields of geology. If we successfully hire a new mineralogist, perhaps crystallography will make a come back.
Several week of instruction required for undergraduate geology majors.
The environmental field is the main career track taken in modern geoscience programs and our's has also fallen to reducing the emphasis on crystallography and gone more toward geochemistry and hydrology
We teach a little in mineralogy but there is no course in our department for advanced training.
At best it is a single page in a textbook on Earth Science or General Science.
Students are ill prepared to effectively study systematic mineralogy and optical mineralogy. Introduction to crystallographic axes and crystal form is not enough for understanding properties used in routine ID. I have seen this both as an instructor and as a worker in the mining industry supervising summer interns. Those with good crystallography backgrounds did better.
Only basics of systematics are covered and no attention to determinative methods.
The curriculum compression (3 courses once taught in depth and now taught in a very cursory manner as one half-assed course) of many schools has seen crystallography all but disappear from nearly every department.
General departmental support for mineralogy is waning.
Mineralogy: The trend now is to open the course with a bit of crystal chemistry, then go into the "basics" of crystallography, and so on. This is unsatisfactory and reduces Mineralogy to a watered-down chemistry course. I am not a crystallographer, but I feel strongly that crystallography must be given emphasis in an undergraduate Mineralogy course.
We cannot cover all the traditional aspects of crystallography in our undergraduate mineralogy course. We do external symmetry, some crystal forms, some crystal chemistry, some polymorphism/transformations, etc.
Teaching hours for crystallography have been cut down to a minimum by the geological community before I took the position. It is virtually impossible to bring them to a normal level before the soon retirement of the most of the present faculty.
My coverage is excellent. I do not believe that is universal.
These days it is rarely taught in mineralogy curricula.
We have a small amount in mineralogy classes and a full course is offered but few take the course.
Many students take no courses with rigorous crystallography.
Only exposure is in the mineralogy course or directly from me if student needs to use the

diffractometer or has a project involving some aspect of crystallography.
In MY curriculum we spend about 4 weeks on the subject (another 4 on crystal chemistry).
Crystallography (at least in mineralogy courses) has lost coverage to subjects more widely needed by geologists. Hence, real crystallography becomes a graduate pursuit.
It's excellent in my classes...
Many Geology departments are changing their undergraduate curriculum to reduce or eliminate completely those aspects of Mineralogy that deal with crystallography, XRD or symmetry.
Enough for undergrad mineralogy.
Crystallography has been largely squeezed out of undergraduate geological curricula; only introductory or cursory attention is given in most schools.
I have chosen good because I do not teach in academia and my undergraduate years ended in 1982. While I was an undergraduate at Rutgers University I feel the Geology department did an excellent job of covering crystallography.
I believe it has been reduced in importance at the few institutions with which I am most familiar.
Only a few institutions have facilities to teach undergraduates. Postdocs with experience are most often brought in from overseas. These sources are drying up i.e. Germany major departments are closing due to lack of student interest and relatively poor job prospects.
Not many universities are teaching crystallography as an individual undergraduate course.
Fair at my institution. Don't know about others.
No real idea what the coverage is, but the grad students don't seem all that well-prepared for it.
It varies widely from school to school. Some have excellent courses, others, like where I went, did not have anything for undergrads really.
Lots of people still think it's an obscure method. They don't realize that current hardware and software put it in the reach of institutions with decent resources. They don't realize how much we depend on it for what we know about structure.
Where I work the undergraduate chemistry majors have one year of geology and an optional undergraduate course called "Diffraction Methods." That is the extent of what is offered to our undergraduates.
Must be site dependent.

Respondents were asked to suggest specific courses where crystallography should be covered in the *undergraduate physical sciences curriculum*:

Senior inorganic chemistry Senior inorganic/ organic lab
Physical chemistry and advanced inorganic chemistry
introductory inorganic chemistry
Inorganic Chemistry (Senior Level) and Physical Chemistry
A brief description in survey course is fine.
At all levels in both the classroom and the laboratory. There is no course in which some crystallography would be inappropriate.

Inorganic Chemistry, Biochemistry
Physical chemistry and/or Instrumental Analysis.
Analytical chemistry Inorganic chemistry
Organic chemistry, environmental chemistry, materials science, geology, chemical engineering
Freshman chem and physics, p-chem, solid-state physics
either an advanced inorganic class or physical chemistry
Freshman chemistry Physical chemistry
Physical chemistry
Advanced Inorganic Chemistry Group Theory
Physics, Chemistry and Engineering majors need basic vocabulary to discuss molecular structure, solution processes, phase transitions, and corrosion intelligently.
General chemistry--along with landmarks in chemistry Advanced inorganic--one to four lectures Physical chemistry--three to four lectures
Physical chemistry, Inorganic laboratory
physical chemistry, inorganic chemistry, organic chemistry
Wave theory, solid state (nanotechnology), material science, etc.
This depends on the depth to which one wants to go. Among the possibilities are: a single lecture in a biochemistry survey course (which is what I do at present), a few lectures in the Physical Chemistry course, and a one semester course of its own.
Introductory Biochemistry (structural biochemistry semester for 2-semester sequences) is where some simple basics can be treated; Other possibilities for crystallography modules might include physical chemistry or instrumental methods, where these might be coupled to laboratory work; Institutions that have a biophysics program might offer a more in-depth elective in crystallography as a part of a biophysics course.
Biochemistry Inorganic Chemistry Instrumental Analysis Material Science Solid State Physics
Crystals, crystal symmetry, x-rays, diffraction
either in biochemistry of physical biochemistry
Any course where structural biology is the key should give a minimum coverage to looking at and evaluating structures. Technical crystallography is not very important to them although the more people who understand how easy crystallization is the better.
Biophysical Chemistry
general, organic, biochem, and physical chemistry, general bio, general physics, material sciences
Chemistry, Physical Biochemistry.
Analytical Chemistry, Physical Chemistry, Intro to Physics
physics of the solid state
Probably not necessary.
Advanced Biochemistry course, Advanced mathematical course, interdisciplinary course between biochemistry/physics/math
Advanced inorganic chem where much of the symmetry is already covered.
Crystallography should be presented as a technique supporting structural biology, similar to protein sequencing, mass spectroscopy, etc
Covered in an Advanced Physics/Optics course.

Impacts on biochemistry, and it also fits well in physical chemistry
General chemistry, physical chemistry, physical organic chemistry, general physics, chemical physics
Physical chemistry, inorganic chemistry
Material Science, Diffraction physics etc
Chemistry Physics
Biochemistry Physics Computation Mathematics
Chemistry/biochemistry, Biophysics
Earth Materials
mineralogy, solid state, materials
Should be taught in introductory mineralogy as part of at least a one semester course. Should also be covered in courses in crystal structure analysis, x-ray diffraction techniques, etc. and courses in gemology.
mineralogy and physical chemistry
Mineralogy and Optical Mineralogy, Methods in Chemistry
In my field, this should be covered in mineralogy, although it could also be covered in a crystal chemistry or materials science class.
Mineralogy Physical geology Inorganic chemistry
In the earth sciences, it should be taught in mineralogy.
mineralogy advance mineralogy sedimentology/sedimentation physical chemistry analytical chemistry quantitative methods in chemistry
Mineralogy, for sure I would like to see at least a little attention given to crystallography in the first-year chemistry sequence. This would enable me to go much further with these concepts in my mineralogy course.
Mineralogy, chemistry dealing with structure of compounds and solid state physics.
Intro mineralogy Petrology Optical courses
General chemistry. Earth Science. Of course, mineralogy and petrology.
Mineralogy Intro Physics - Optics Intro Geology Intro Chemistry
solid-state physics, chemistry, geology, biology
Materials science Mineralogy Elementary and Advanced Physics Courses Elementary and Advanced Chemistry Courses
Mineralogy Diffusion and mineral kinetics Structural geology
Physics (1st year), Chemistry (1st year), Mineralogy, Materials Science (1st year), and many advanced courses.
Introduced in Mineralogy, covered in more detail in any upper level Mineralogy or crystal chemistry courses take as electives by undergrads.
Chemistry, physics, geology all should offer some elements of crystallography as required of undergraduates. it is pointless to specify courses given diversity of offerings
Earth Science, Geology, Physical Science, General Chemistry
Prereq for systematic mineralogy and optical mineralogy. I have taught a subset of crystallographic concepts to non-major undergrads in labs for Gems and Gem minerals (If art majors can understand it ANYBODY can!) Something should be taught in the sold state chem sequence, but I am a geologist, so not sure where.
Basic material science; Advanced topics in inorganic and chemistry; mineralogy (separate course); Biological materials

within geology curriculum: mineralogy and petrology at undergrad level and crystallography or structural mineralogy at grad level
Maybe chemistry, some in mineralogy, but that's it.
Introduction to geological materials Mineralogy Mineral identification (X-ray diffraction)
Crystallography, physical geology, optical mineralogy, geochemistry, igneous petrology, structural geology
Should be basic to courses in the solid state
Mineralogy, geophysics, solid state physics
Mineralogy, materials science, chemistry, physics
Some aspect of all of the disciplines: geology, chemistry, biology, physics.
College chemistry Mineralogy Optical mineralogy Solid state physics
Elementary Mineralogy
Mineralogy, petrology
Mineralogy, Petrology, Optical Mineralogy lab, Crystal Chemistry, probably more but these are all I can remember from my narrow background.
Mineralogy and petrology (for geosciences, my background); solid-state (condensed-matter) physics, materials science, metallurgy, nanoscience
Materials science for engineers, crystallography and mineral science for geologists, crystal physics in 2 semester physics
Solid State Physics, Materials Science, Chemistry and Pharmacy.
Physical chemistry laboratory condensed-matter physics mineralogy
Some basic level courses should e covered as separate courses or may be included with higher level physical chemistry courses
Should be covered in Physics: Intro and solid state Chemistry: intro and group theory Earth Sciences: should be covered in depth in mineralogy class Materials Science: should be covered in depth
General Chemistry should have an introduction to crystallography. Our sequence includes a small section on crystallography, but I feel it is inadequate. Inorganic Chemistry does a good job of dealing with symmetry and usually seems to cover a small amount of crystallography. Mineralogy usually does a good job of covering crystallography. I think students leave with a good sense of where the atoms are in natural crystals. They usually have a reasonable understanding of symmetry at the end of such a course. I think it's easy to transfer this material to synthetic / materials systems.
Introductory structure of materials, solid state physics, inorganic chemistry
Intro to Chemistry Inorganic Chemistry (jr. and sr. level) Analytical Methods
I think there should be basic coverage in intro chem (or at least inorganic and organic chem), physics (ditto for solid state), and mineralogy. Each discipline could have a course specially designed to address crystallographic concerns within its scope. And a general crystallography course that is available to all would be an excellent idea.
At some level, it should be touched on in general chemistry (most texts do crystal structure and Bragg's law, but give really little insight into how diffraction patterns and structure are related; organic chemistry (I don't thing most texts do much with it); biochemistry (most texts have a mystifying page or two on the subject); physical chemistry (treatment depends a lot on the individual - crystallographers teaching PChem include it, non-crystallographers don't, is the rule). It would make a great application for Fourier series in calculus courses.
Chemistry and Biology. I assume Physics students learn diffraction theory.

Brief overview in class and inclusion of solving structures in inorganic or organic labs
Crystallography should be covered at introductory level in introductory courses in all physical sciences. In advanced coursed, it should be covered at the relevant level in the relevant courses, including organic chemistry, inorganic chemistry, physical chemistry, materials science, and analytical chemistry.
1st physical chemistry, quantum physical chemistry, special topics course in structural methods, preferably as a lab

Respondents were then asked to suggest the depth of coverage/topics to be covered in crystallography in the *undergraduate physical sciences curriculum*:

Hands on approach to crystallography without going into details of theory (similar in depth to NMR or Mass spec)
Space groups, direct methods, use of the Cambridge data base and use of model drawing software (such as mercury).
the diffraction phenomenon, unit cells, symmetry, mineral structures, unit cell contents, chemical formulas, bond distance and angle calculations, symmetry, systematic absences
Limited to one week worth of lectures. General survey of topics.
I do not advocate a course of any depth in undergrad training
Crystal growth and full structure determinations should be a part of every student's experience. Also, crystallography is an excellent introduction to practical applications of symmetry.
Intro to crystallography, i.e. what the technique is, how it works, and why it is useful.
Basics of X-ray diffraction, e.g. the Bragg equation, unit cells AND SYMMETRY, intro to space groups and how structures determined - briefly.
Basic introduction to the technique, its vocabulary, and its limitations.
Powder diffraction is a relatively concise topic that could be taught in a number of programs of study. Students could gain enough understanding of this subject in fewer contact hours than for single-crystal methods. The issue is giving the students something of value they can use in other facets of their studies. Powder diffraction has applications in many fields.
Basic diffraction theory as well as application
A brief survey of how xtal structures are solved plus a deeper introduction to space group symmetry.
Depth of coverage: Students should understand the basics of diffraction, X-rays, the crystal mosaic and reciprocal space. If possible, they should have some hands-on experience and learn how the common solution programs work. They should grow crystals of small molecules and solve at least one structure on their own.
Crystal growth and full structure determinations should be a part of every student's experience. Also, crystallography is an excellent introduction to practical applications of symmetry.
Lattice points (of identical environment) Unit cells of lattices 7 crystal systems (distinguished by symmetry and its consequences) Lattice centering (P,I,F,A,B,C) 14 Bravais lattices Screw axes and Glide planes (new 2-part symmetry elements) Graphical symbols for all symmetry elements in any orientation in 3D Hermann-Mauguin symbols for all symmetry elements/operations Fractional coordinates x,y,z Algebraic expressions for applications of symmetry operations 230 Space groups and International Tables depict-

ing how they work Multiplicity of atoms placed at a general position x,y,z Equivalent positions Multiplicity of atoms placed on special positions (symmetry elements) Asymmetric unit The number of atoms/molecules in a unit cell and in its asymmetric unit Miller indices hkl as descriptors of stacks of planes slicing the unit cell Inter-atomic distances, Bond angles, Torsion (dihedral) angles, Planar groups of atoms, Packing diagrams, H-bonding networks, atomic displacement parameters, bonding electron density and lone pairs.
Famous crystallographers and Nobel Prizes Types of solids--ionic, molecular, polymeric, etc. Some idea of the results that can be obtained from the crystallographic experiment and how it is carried out. In physical chemistry the idea of space groups should be introduced.
Basic coverage so they can understand the application to structural work. Much the same level as is used to cover NMR so it can be used for structural work.
brief introduction to the methods, some fundamentals, if possible, some inclusion in laboratory
relate the structure to function (kinetics) and thermodynamics, whether structure of the elements, compounds, or molecules (ionic or covalent)
Introduction to the principles of crystallography; brief treatment of symmetry and space groups; explanation of the methodology used to create protein structural models from experimental data; evaluation of the quality of structural models; visualization of x-ray structures in the context of experimental functional data.
Biochemistry: 1) methods for crystallizing proteins. 2) different instrumentation and requirements for protein work 3) discussion of moving from primary sequence and electron density data to structure data 4) downloading and displaying structures in the PDB 5) using crystal structures to identify amino acid side chains involved in catalysis and to propose reasonable mechanisms for catalysis. 6) Demonstrating the effects of ligand and substrate binding on the tertiary structure of proteins (conformational changes induced). Inorganic should include a theoretical basis for the technique, along with some of the mathematics to go from scattering patterns to 3D structures.
More on the basics of space group determination
At the undergraduate level, only the most theoretical understanding of the geometry should be taught. i.e., no proofs with Fourier transforms at that level.
why diffraction, what you get and why, limits of results, interpretation, etc.
Bragg law, electron density etc.
sufficient general explanation to convey the principals involved & allow the student to properly interpret the results of such experiments
As deep as possible
None - the field is too specialized and mainly a technique no more important than electrophoresis or chromatography.
General knowledge of how to determine a structure beginning with a protein of interest For end users only: how to assess the quality of a structure and general concepts on how to interpret a structure [identifying motif/folds, active sites, binding sites, etc.]
Symmetry, basic diffraction theory. Anomalous absorption edges could be taught as part of a spectroscopy course.
Understanding where the information that goes into an electron density map comes from. Non crystallographers should have a working understanding of the process so that they can form judgments about the quality and accuracy of structural data which they encounter in their work.

Minimal depth. Summary only
Should be a major topic of a Physics/Optics class.
What it is, what it gives you, inherent assumptions involved (i.e. that it is a static view).
Focus on diffraction, including topics such as anomalous, synchrotron and laser diffraction (and ancient topics such as neutron diffraction), and symmetry. Also discuss atomic and small-molecule geometry and electronic structure as revealed by crystallography and how this correlates with related fields such as atomic theory, scanning probe microscopy and electron microscopy.
See item 6 above. Topics? Everything needed to solve a structure. Standard syllabus should include topics covered in books by Buerger, Dunitz, Woolfson, Phillips, Evans etc
Enough to understand space groups, indexing, refinement Fourier theory
How to obtain macromolecular structures How the X-rays diffract, what information can we extract from X-ray data from a crystal. Space groups Symmetry
I would give an overview of the whole process, spend some time on diffraction and space groups, and on solving the phase problem. Spend less time on refinement.
symmetry, point groups, space groups
Introduction to both theory and practice of crystallography.
A rather open-ended question for a survey. I think that only a little crystallography is needed by geology undergrads.
Basic treatment of symmetry (point, plane, space), some matrix algebra, perhaps Fourier transforms, definitely some diffraction theory beyond Bragg's law.
crystal classes symmetry elements
Symmetry, symmetry notations for crystal classes and space groups, nomenclature for positions of atoms in a structure
identification of minerals by X-ray diffraction
depends upon curriculum demands –
Coordination; point group and plane lattice symmetry; a nod to space groups, including some coverage of 3D symmetry operations. I am pleased to have available software such as Xtaldraw which make it possible to present a lot of material visually. I think few undergrad geoscience students will be either interested in or well-prepared to do transformations, solve crystal structures, etc.
At least to the level of introductory space group material.
crystal systems, symmetry, point groups, space groups
Morphological crystallography, point groups, crystal growth & reactivity.
Crystal symmetry, Coordination crystal chemistry, Major crystal structures in relationship to physical properties, Crystal growth, Crystal deformation mechanisms
Basic structural identification, typism.
In all of them sufficient understanding should be taught in order to recognize where a deeper understanding is needed as it might apply to the subject matter of the field.
Symmetry concepts Elementary crystal physics Common crystal structures Interaction of radiation with matter
Mineralogy: symmetry (symmetry elements, combinations in point groups, lattices, and some mention of space groups), forms (symmetrically equivalent faces), Miller Indices
intro to symmetry, lattices, point groups, concept of space groups, Miller indices
lattices, point groups, introduction to group theory
Crystal systems.

symmetry elements, crystal systems, crystal structures relevant to the discipline, should be covered a minimum of 5 weeks of instruction
minimum of crystal systems, classes and symmetry operations
For most geology students crystallography will be of little help in their careers
At a minimum: Bravais groups, symmetry elements and crystal forms.
For those who need it: Crystal systems, x-ray diffraction and powder techniques for compound ID, crystallographic controls on physical properties (save optical properties for another course), determination of unit cell parameters and cell refinement for isometric system.
Should be able to demonstrate ability to perform simple structural analysis and simulate XRD patterns.
All basic topics of external and internal crystallography including optical microscopy and crystallography, basic symmetry and introduction to space groups, basic x-ray diffraction
enough so that students understand the space groups and what they represent in terms of actual specimens in, for example, an XRD pattern.
Stop at the 230 space groups.
bonding, ionic radius, lattice planes, miller indices, unit cell,
crystal lattice (basic geometry) -crystal symmetry (introduction to point groups and space groups) -elementary crystal chemistry -powder diffraction method (introduction to the identification of minerals)
Crystal lattice and crystal structures. Substitution. Diffusion. Space groups.
Through some understanding of space groups and diffraction theory
Crystal systems, classes (point groups), space group symmetry.
basic crystallography (in order to relate it to optical mineralogy and petrography)
Principals of X-ray diffraction--instrumentation, mechanism of diffraction, use in determining crystal structures (qualitative) Crystallography--symmetry, space groups, Miller indices, atomic coordinates, drawing crystal structures
I cover xtl systems, point groups, plane groups and then relate them all to real minerals, linked with XRD work.
Bravais lattices Point group symmetry X-ray powder diffraction Working with the results of crystal structure determinations (lattice parameters, interrelationships among structural and chemical parameters, etc.)
Up to and included the 32 crystal classes
Symmetry as far as space groups, XRD powder methods, systematic mineralogy, crystal chemistry
symmetry, crystal systems, point groups, space groups
moderate depth = significant portion of one-semester course
diffraction physics, point groups, space groups
I would want the students to have a very strong background in math so that basic crystallography could be introduced using vectors and linear algebra. It makes further development of reciprocal space much easier.
full development of the 230 space groups, crystallographic controls on phase transitions and phase stability, relationships among thermodynamics and crystallographic concepts (e.g., symmetry/entropy)
crystallography of phase transitions, crystallography of ferroelectrics and high Tc superconductors, biomaterials

A course on x-ray crystallography covering single-crystal methods, powder methods and x-ray fluorescence analysis.
crystallization, simple kinematic diffraction, (space groups) symmetry, examples of solved structures, interpretation of graphic presentation
As indicated in previous question (point 7), basic level will be recommended.
Students should understand the difference between an amorphous and crystalline material. Crystal structures, in my opinion, should be taught using polyhedral models, which make it easier to see linkages and patterns. I am not in favor of having students memorize a bunch of crystal structure, but if handed a crystal structure, they ought to, for example, be able to determine the oxidation state of a transition metal cation in that structure by looking at the model. Furthermore, I think they ought to receive some introduction to the link between properties and structure and an introduction to defects.
Ability to understand structure factor of ordered crystals, related reciprocal space to symmetry etc., understand Fourier transform. Link symmetry and structure to physical properties
Intro -- Fact of its existence, Bragg's Law. Inorg Chem -- Nature of crystallographic derived data, potential pitfalls of x'al data. Anal. Methods -- Brief overview of techniques, critical analysis of results.
Crystal systems, space groups, symmetry, x-ray diffraction.
Somewhere in a chemistry curriculum, cover Bragg's law, unit cell dimensions and structure as Fourier transform of structure factors, phase problem (geometric solutions), and especially at any level, JUDGING THE QUALITY OF CRYSTALLOGRAPHIC MODELS.
Diffraction theory, applications of crystallography to problems in Chemistry and Biology, the problems involved in obtaining crystals and final structures
Nothing too deep - much easier to learn the theory after solving a few structures
General chemistry: Introductory and general material. Organic Chemistry: How to look at an organic structure determination. Inorganic Chemistry: How to understand the results of an inorganic structure determination. Analytical Chemistry: Instrumentation. Physical Chemistry: In-Depth coverage of scattering methods in general. Materials Science: Overview of all available scattering methods.
Bragg's law, reciprocal space lattice, powder diffraction, single-crystal diffraction, Fourier transform, refinement, preferably as a lab or hands-on computer based course.

Respondents suggested the following courses where crystallography should be covered in the *undergraduate life sciences curriculum*:

physical biochemistry
None.
A brief description in survey course is fine.
Biology--protein structure.
Molecular biology.
Biophysics, pharmaceutics, microbiology
Freshman chemistry, beginning biology, more (but I don't know their names).
None
structural biology
Protein structure/function.
Molecular biology was founded on crystallography and a majority interest will continue to be in structure/function relationships. Intelligent discussion must assume knowledge of

those same basics concepts already listed in 8. above.
No progress would be made in biochemistry without crystallography. I'm not sure what the courses are called.
molecular biology, biochemistry, biotech
Any fundamental course dealing with DNA, RNA, or proteins and function.
This is harder than for physical sciences, as the students generally lack quantitative background. That makes it hard to handle crystallography. It could be done, but a few lines in a survey are not enough to cover the question.
Much the same courses as mentioned above for physical sciences.
Biochemistry (I don't think most biology departments would be able to provide a useful course-better to avoid it than do a poor job covering it without sufficient expertise to do a good job).
Biochemistry, physical chem.
Biochemistry or Pharmacology, perhaps biology
general biology, molecular biology
Physical Biochemistry
Intro to Biochemistry, Advanced Biochem
Biochemistry
Biochemistry
Zip.
Biochemistry
Biochemistry
Crystallography should be presented as a technique supporting structural biology, similar to protein sequencing, mass spectroscopy, etc
Certainly Advanced Biochemistry and/or Biophysical Methods. At least touched on in Biochemistry.
intro to biochemistry, biochemistry II, physical biochemistry, cell signaling,
biophysics/biophysical chemistry
At least the courses in Molecular Biology and Biotechnology.
Biochemistry Molecular Biology Cell Biology Pharmacology
Molecular Biology
Biochemistry
General biology and beyond -- not methods in detail but the nature and importance of the results.
Biochemistry
would be nice to see it addressed in any course in the biology group
Molecular Biology
molecular biology, paleontology
in a biochemistry course or organic chemistry course
Biochemistry
No background to provide an answer. However, most biology departments are NOT EXPERTS in crystallography; these courses should be in earth science, material science, or chemistry departments. We should encourage diversity by not expecting every department to teach their own version...when I want to learn statistics, I go to the math experts, not the biologists!

biological materials (proteins, viruses, macromolecules, bones and teeth)
Beginning biology should point out the gains made by understanding the crystal structure of complex organic molecules. Additional development within courses dealing with the functions of these complex molecules.
None
biomineralogy, protein crystallography, nanomaterials
protein structure, enzymology, genetics
Don't know. Perhaps as part of a methods course? W/x-ray diffraction?
Similar to that stated above -- particularly for organic chemistry and biochem.
Biochemistry.
Essential diffraction theory (with only the necessary math in some classes), crystallization of macromolecules and the problems involved (e.g. preparation of proteins for crystallization), applications of crystallography in biology (i.e. basic structural biology)
General Biology, Molecular Biology, Molecular Genetics
possibly in a special topics course for structural biology or structural biochemistry

Respondents were then asked to suggest the depth of coverage/topics to be covered in crystallography in the *undergraduate life sciences curriculum*:

the diffraction phenomenon, unit cells, symmetry
I do not advocate a course of any depth in undergrad training
Intro to crystallography, how it works and how it is useful.
As much as a faculty member can get away with. Only those faculty with research projects in macromolecular crystallography will generally give any time to crystallographic topics.
As above, except for the growing of crystals and structure solution. They should work through, as a group, one structure solution for a biological molecule. They should understand chirality and how it affects structure solution. (and from that point of view, they could grow crystals of small molecules and solve the structures.)
As in 8. above but there will be resistance to 3-D thinking from those students less mathematically able. (Often the reason otherwise good scientists go into biology in the first place.)
brief introduction to the methods, some fundamentals, of possible, some inclusion in laboratory
concentration on protein structure, function, and mechanism
Same as above for physical sciences.
For those courses, the main focus should be on accessing crystal structures, thinking about them, and understanding the statistics well enough to know how reliable a given structure is.
why diffraction, what you get and why, limits of results, interpretation, etc.
Basic concepts of pros and cons of the method.
sufficient general explanation to convey the principals involved & allow the student to properly interpret the results of such experiments
Deep enough
General knowledge of how to determine a structure beginning with a protein of interest For end users only: how to assess the quality of a structure and general concepts on how to interpret a structure [identifying motif/folds, active sites, binding sites, etc.]

Biochem should say something about the nature of protein crystals so students can relate PX results to studies in solution.

Minimal depth. Summary only

Should be a major topic of Advanced Biochem/Biophysical Methods. Brief coverage (e.g. 1 day) in Biochemistry.

A critical appreciation of the results of crystallographic (and NMR and theoretical) studies is an essential skill for consumers of structural information--what can be inferred from a given structure and to what extent? Students must be trained in how to use tools to explore and analyze 3D structures and understand that there are methods to predict a structure by extrapolation. They must understand macromolecular structural components (post-translational modification, 2nd struct, topology, domain architecture, 3D shape, multi domain construction, quaternary interactions), how these structures move and how they interact with ligands or substrates. Finally, they must be trained in how to integrate this information into a picture of the whole cell (a la, Goodsell's "Machinery of Life").

Stryer, Voet & Voet, Branden & Tooze

Ways round the phase problem in a descriptive sense Ability to display and understand a PDB file

Not too deep - should cover the basic principles, and spend a lot of time on the results (the structures) since those are more interesting to undergrads in the life sciences. If they want to learn more about the techniques, they will get a chance later on.

Visualization of a few illustrative macromolecular structures with challenges on structure-function relationships should be part of any molecular biology, cell biology, or biochemistry course.

will not happen

introductory

In all of them sufficient understanding should be taught in order to recognize where a deeper understanding is needed as it might apply to the subject matter of the field.

3 weeks minimum on crystal structure

Organic crystallography and the importance to elucidating protein structures, etc.

Same as question 8, but with emphasis on biomaterials

Relationship of crystallography to strength of "hard" tissues (bone, teeth).Relationship of crystallography to various "stones", like kidney stones.

diffraction physics, point groups, space groups

biocrystallography, crystallography and biofunction

interpretation of graphic presentation

There are a lot of crystalline materials in many organisms (bones and teeth), so an introduction to crystallography and biomineralization is certainly appropriate. I don't feel that a great amount of depth is required in this field.

General nature of diffraction, relationship of diffraction data to unit-cell dimensions and structure, phase problem, JUDGING MODEL QUALITY.

I would follow the list of topics in the book by Glusker and Lewis: Crystallography for Biologists and Chemists.

General biology: Introductory material. Molecular Biology: How to understand the results of a structure determination. Molecular Genetics: How to understand the results of a structure determination.

similar to graduate level: familiarity with Bragg's Law, resolution limit, R values, enough to understand the limitations of the method and to be able to evaluate the quality of work presented in a structure paper

Respondents made the following comments with regard to coverage of crystallography in the *graduate curriculum*:

My own lecture ;-)

Offering of crystallography courses here is spotty at best. I usually send my students to workshops off campus for training.

Usually there is either a three credit course or a 1 credit course in crystallography at most schools. The 1 credit course is usually a "hands-on" how to do rather than theory. Most students want to get things done and are happy with the ORTEPS and data tables. Tweaking of the data is not what students are interested in. Hence, the training tends to meet the needs of the students.

There is training available to those so inclined.

Only a few inorganic chemists ever receive any formal training. Organic chemists almost never use crystallography because it is not a part of their education.

Best class I have taken in grad school.

Very few universities have faculty who are competent to teach X-ray crystallography.

Very little is taught even though the technique is widely used.

It is particularly well-received here at the University of Minnesota. An average of 10 graduate students annually completes a blended theory and practical course in X-ray crystallography where each must collect their own data, solve and refine an unknown structure and prepare publication materials. This makes more sense than teaching theory-only courses.

Twenty or so grad students take the crystallography course, mainly those in groups that do lots of synthetic work. The course gives a decent background but nothing in depth.

There are no specific classes in the chemistry department. There is an inorganic spectroscopy class which covers crystallography for one week and there is a powder diffraction class offered in the materials science department.

There is a 15 week course with hands on experience.

Depends on who's teaching, how much hands-on experience the students get etc.

For pending practitioners excellent in some places but haphazard in others. Many practitioners trivialize subjects because they don't know better themselves.

The courses that are offered are somewhat limited in scope.

Need at least one term full course in diffraction theory for any student in crystallography.

Except for those students whose research is in crystallographic labs, very few learn it at all.

Unless you are a student studying crystallography, not much gets passed on.

Probably insufficient coverage unless the chosen field of expertise directly requires some experimental crystallography.

There is one 1-credit course offered during the year.

Wish they would teach more about the practical theory, i.e. what shortcuts the software programs are taking, more on crystallographic computing.

I felt that the theoretical understanding of the math in crystallography was too separated from the application.

In major centers for crystallographic graduate training, such as Purdue University and others, I think those who are interested can get good training. At universities where there are few crystallographers, training may vary and may depend on the individual to ac-

quire.
This depends on the institution and on their major. We have two graduate classes of 8 weeks each on protein crystallography. Even this is not adequate.
This answer is an average of excellent (for those students who pursue crystallography as their primary graduate focus) and poor (for those students who choose another path - and are then left generally uninformed about crystallography).
The courses I had were sufficient for me to learn crystallography as I was doing it.
Not enough depth and theory...too much reliance on canned programs.
Only few students are exposed to crystallography during graduate school.
Some departments have decent programs; others, poor to useless.
Not much better than for undergraduates.
Only one course!
This often depends on a students chosen area of expertise. Structural biology graduate students most likely will take an advanced course in crystallography.
Depends on where you are and who the crystallographers are there. Very variable.
At my institution, when I was a graduate student, there was available only an introductory course combining nmr and crystallography.
Efforts are being made- but not many students are actually interested. I think this also varies greatly by school such that the more crystallographers on campus, the more it is covered in lectures. At a minimum, I feel that all research students should be knowledgeable enough to evaluate structures in the PDB and published papers. Often at seminars I have seen more advanced researchers in other fields, such as cell biology, interpret their data based on a crystal structure. They make no mention of the quality of this structure, and indeed for the few I've checked up on the structures were barely acceptable and should not have been used to extrapolate the points made in the seminar.
At the graduate level, students in crystallography programs are well trained but it is the other biology students who need to be trained as intelligent consumers of structures. As is, they tend to trust the crystallographic (and NMR based and even theoretical) models as gospel.
The classes I've seen taught are too watered down to be of practical use to beginning students in crystallography. There seems to be a fear of introducing biology students to mathematics and physics.
We have several crystallography classes in the graduate curriculum here at the UW. We cover the material OK, but whether we do so effectively is another question.
In general not enough courses of theory are provided to have a good background. Most students do not have enough math courses to understand the math behind the computations involved. In general only physics students tend to have enough math and lack the biological background that if willing seems easier to remediate.
I believe that biochem here has excellent courses on crystallography, but the bioinformatics students don't generally take them. They usually take a course on protein structure and one on protein-structure prediction, but not an experimental course.
At my university we have no macromolecular crystallographer, and only one course that deals with macromolecular structure at the grad level.
Coverage depends on what the student is planning to do with his/her life. Coverage will be student dependent.
Typically required only of those taking advanced mineralogy and/or courses in x-ray identification.

Some schools still provide this - my institution does not.
Most of our graduate students are introduced to crystallography in a course on Structure of Solids. Only those performing single crystal structure determination received more instruction. No course on X-ray crystallography is currently offered.
We no longer have an analytical techniques course where training is provided.
It seems that there has been a trend towards decreasing the hard, fundamental sciences in the past 20 years.
Non existent.
Most graduate students in the earth sciences would collaborate with a professional crystallographer rather than learn the crystallography themselves.
Better courses offered at the graduate level.
At this university I am one of two hard rock faculty. With equipment constraints and direction of more coastal geology and environmental geology in graduate curriculum can only use powder diffraction for mainly clay mineral investigations.
I think it is very uneven. I think a large proportion of grad students in geology get no additional crystallographic training at the graduate level. Clearly some programs are strong and attract students in crystallography, but these are few and far between. I think crystallography is neglected in a lot of places.
Few courses in our graduate curriculum deal with crystallography. Coverage is excellent in those courses that deal with crystallography.
It's not required in most graduate curricula.
Again - The two institutions I have been affiliated with as a faculty member (a large research school and a more comprehensive institution) have both cut crystallography and optical mineralogy/microscopy from the graduate curriculum.
Non-existent, except at grad schools where crystallography is used regularly in research projects.
Again, it is up to students to take appropriate courses. The crystallography courses offered are excellent.
Poor. This is my suspicion based on what I see around me.
Varies greatly from institution to institution!
There are very few -- if any -- graduate-level courses in this topic. Students learn techniques/concepts on their own and by interacting with faculty/researchers.
It is available in other departments on campus as needed for individual students. No emphasis in our department at present.
Clay mineralogy is the only graduate course that deals with crystallography.
Almost nonexistent.
There is none in our graduate curriculum.
It varies. Some institutions have all but phased out the "hard" component of a geosciences degree.
With the two graduate programs that I have experience with, it was assumed that crystallography was taught at the undergrad level. There were no graduate Crystallography courses available.
No formal course work is provided.
Ditto. For example, at our school, chemistry has one foreign trained research assistant professor who does all the crystal structure determinations for the whole dept. The students know a lot about the principles, but almost nothing about how to do it.

General departmental support for mineralogy is waning.
It's getting worse as the new wave of students in Geology have had nearly no crystallography as undergraduates.
There is no advanced coursework in crystallography in our department other than clay mineralogy.
We are doing our best on this level, but the bachelor level on geology is too poor.
Not very good.
Depends on specialty.
Only those who specialize take any crystallography.
It's very good, as long as the students take the courses offered!
The only coverage in the Department of Geosciences is in a Grad-level course on powder XRD methods unless a student takes a Special Topics course involving crystallography from me.
Depends on the needs of the students whether they should have more or less.
The coverage is good, but the numbers of students who take crystallographic courses at my institution is small.
We do not have a Mineralogist on our faculty at present.
Don't teach it.
When available at graduate level, it is generally very good -- though typically taught in departments other than geology.
Both the Chemistry and Ceramics departments at Rutgers University give excellent coverage of crystallography in their graduate curriculum. I took courses in both departments to earn a masters in 1999.
Most departments (with which I am familiar) offer a reasonably advanced crystallography course.
Similar to 4 with many older crystallographers retiring. It is not always easy for people to get to synchrotrons and groups tend not to be always open there.
Not many universities are teaching crystallography as an individual graduate course.
There is none, as far as I know.
In Materials Science and Mineralogy, I think the crystallography coverage is good to very good. In chemistry, I think the crystallography coverage is fair to good. For the most part, I feel that those students and post-docs who demonstrate strength in this area have obtained that knowledge on their own - through their research projects.
The graduate course in Crystallography covers both theory and practice in the period of a semester and provides a solid background. In addition other courses emphasize the utility of crystallographic information.
Once again, the same answer. The crystallography I needed in grad school I had to teach myself because there was no formal course at my school.
I don't know from direct experience. I meet more graduate students at meetings who are getting crystallography experience even though they are not crystallographers. That's a good sign. That's about all I have to go on.
We offer one 30-hour course on crystallography for graduate students.

Respondents were asked to suggest specific courses where crystallography should be covered in the *graduate physical sciences curriculum*:

Solid State Physics/ Chemistry
Advanced Inorganic Chemistry A course on applied structural methods (IR, NMR , X-ray)
generally this is done here as a special topics course offered occasionally, or part of an inorganic course in instrumental analysis
If the material is not taught as a specific course then in a Structural Methods Course (Inorganic or Organic)
A graduate course focusing on crystallography including laboratory can be well represented in a one semester grad course.
Virtually all courses. Best to begin with a practical level course in hands-on crystallography and get everyone to do at least one structure.
It should be a separate course on its own at the graduate level.
Separate one semester course in X-ray crystallography with adequate hands-on examples.
Should be covered as a separate course or part on inorganic chem. The problem is most chemists are unable to teach it.
Geology, inorganic chemistry, solid-state chemistry, chemical engineering
specific courses in crystallography in Chem, physics depts.
Inorganic, organic, physical, analytical, and perhaps even polymer. I think it is a basic tool that all scientists should have an understanding of
Inorganic chemistry Organic chemistry Specialized course in crystallography
separate courses in our curriculum
There should be a course in X-ray crystallography, devoted to small molecule structures. X-ray diffraction and materials science X-ray powder diffraction
Virtually all courses. Best to begin with a practical level course in hands-on crystallography and get everyone to do at least one structure.
The % of publications including the results of organic and inorganic crystallographic analyses is now so high ALL serious researchers in these fields should be able to assess them critically.
In Chemistry and Biochemistry departments a full course of crystallography should be offered--a minimum of one quarter or one semester. In Physics and Geology a course should be offered that would be tailored to those fields.
General coverage of crystal systems, space groups, solution techniques, and refinement
inorganic chemistry, organic chemistry
should offer a full course of diffraction theory and determination of protein structure by nmr, spectroscopy, and crystallography
Any graduate level course in biochemistry or macromolecular structure should have some component of crystallography.
small and macromolecular structure determination
biochemistry, protein crystallography
Biophysical chemistry or Biophysical techniques
All physical methods courses in the graduate curriculum should have some detail about the method of crystallography.
Biophysical chemistry, physical chemistry, structural biology. Mostly courses geared towards structural techniques and results.

Any core chemistry course.
Analytical Chemistry, Physical Chemistry, Physics, stand-alone course: Crystallography
X-ray structure analysis Practical crystallography
mathematics used in crystallography, course on phasing, course on modeling/refinement protocols AND a course on model validation and ethics
Some understanding is useful for med chemists.
general core class - advanced topics course
Inorganic chemistry, analytical chemistry, solid-state physics.
It should be taught in the research environment
Almost all courses could benefit from crystallographic inclusion. However, teaching the basics should be relegated to something like biophysical techniques, while evaluating the structures should be presented to all students in a beginning course.
Physical organic chemistry, condensed matter physics
biophysics, structural biology
In specialty courses.
Crystallography should be covered as an independent course per se.
Advanced Mineralogy
advanced mineralogy, x-ray crystallography, techniques and or instrumentation courses
Structure of Solids, X-ray Crystallography
X-ray Crystallography, Analytical Techniques
A student of mineralogy should be able to take at least one course dedicated specifically to crystallography, where geometrical crystallography, crystal structure analysis, and diffraction physics are covered at an advanced level.
Analytical methods in mineralogy
In the earth sciences: advanced mineralogy and petrology
crystallography applied instrumental methods
see undergraduate section - also depends upon graduate program offerings
I have assumed that most crystallographic training at the graduate level occurs within courses focused on crystallography and crystal chemistry. I assume that there will be some inclusion of crystallographic concepts in ig and met petrology courses.
Same answer as for undergraduate except covered more deeply and in a more detailed manner.
mineralogy, materials science
Advanced mineralogy/crystallography. Could be combined between physics, chemistry, geology, materials science.
Crystal chemistry Mineral textures
Crystallography of minerals
petrology, mineralogy, solid-state physics
Advanced mineralogy, crystallography in geology.
Advanced Mineralogy Advanced Petrology
advanced mineralogy, clay mineralogy, x-ray diffraction, transmission electron microscopy
Advanced mineralogy or crystallography courses. X-ray diffraction techniques.
varies by discipline
optical mineralogy

x-ray diffraction techniques and methods, crystal structure determination (x-ray, electron diffraction, and synchrotron); rietveld and other modern methods of analysis
undergrad and grad courses in physical chemistry and organic chemistry; crystallography in geol. or physics or chemistry or material science
Mineralogy, Phase Petrology, Igneous Petrology, Metamorphic Petrology, etc...
Systematic mineralogy Crystallography Advanced diffraction methods Electron microscopy
Any solid state specialty
Mineralogy, geophysics, seismology
Earth science, chemistry, materials science, condensed matter physics
Course in X-ray crystallography and crystal structure determination
Graduate mineralogy curricula (courses specifically in crystallography) Graduate chemistry curricula (courses specifically in crystallography) Graduate solid state physics
Only as applicable
Crystal Chemistry, Advanced Mineralogy
specialty course
geology, chemistry, physics, materials science, biology
Physical Properties Of Crystals, Elementary Crystallography, Single Crystal X-ray Diffraction Lab, Crystal Chemistry, Inorganic Chemistry, Transmission Electron Microscopy, TEM Lab
crystallography of phase transitions, crystallography of ferroelectrics and high Tc superconductors, biomaterials, group theory
Solid State Physics, Materials Science, Chemistry and Pharmacy.
separate crystallography course
depends on research needs of student
Examples I can think of: Materials Chemistry (major), Solid State Physics (minor), Inorganic Chemistry (minor), Advance Mineralogy courses, X-ray Crystallography (beyond organic crystals, if taught in a Chemistry department), electron microscopy....
Crystallography Course. Solid State Physics Course Structural Biochemistry Course
Advanced mineralogy and crystallography. Analytical techniques.
Any structural biology course should provide guidance in using crystallographic models wisely.
It should be a dedicated course: Crystallography for Physical Sciences
Inorganic classes
For chemistry graduate students, there should be a complete course on diffraction methods that covers all aspects of diffraction as it relates to chemistry.
Special topics course preferably with hands-on computer work.

Respondents then suggested the depth of coverage/topics that should be covered in crystallography in the *graduate physical sciences curriculum*:

space groups, direct methods, analysis of Fourier maps deformation density use of the Cambridge data base and use of model drawing software (such as mercury).
this varies widely depending upon the students taking the course: symmetry, space groups, systematic absences, unit cells, coordinates, Miller indices, geometry calculations, relationships between space groups, diffraction experiment, explanation of normally reported crystallographic data collection and refinement parameters, basic meth-

ods in structure solution and refinement, disorder, partial occupancy, etc.
About two weeks worth of material in a separate course or 14 to 15 lectures (one per week).
Quite a lot of depth, including individual lab studies on real crystallography problems.
Should be very in depth and very hands-on.
Students should understand the overall process and be able to critically read a journal publication containing X-ray structural results.
Students should be able to perform a structural analysis and critique reports by others.
One solid crystallography course is offered at the University of Minnesota, which may be attended by any undergraduate or graduate student given interest.
Introductory and advanced topics -- two courses.
I suggest that there be a class specifically for crystallography from which topics may be covered in detail
In addition to that covered in the undergraduate courses listed above (because not all students will receive that as part of their undergraduate education), they should have a full understanding of the phase problem and mathematics behind structural solutions. They should look at more recent (and more common) problems like twinning. They should solve at least one "normal" small molecule and one with a difficulty, such as disorder or twinning. Materials/mineral structures could be covered in another course, as could powder diffraction and obtaining structural data from powder data.
Diffraction of X-rays modeled by Bragg as reflection from stacks of Miller indexed planes Transforming the spatial distribution of the diffracted beams to yield the unit cell shape, size and orientation. Transforming the intensities I(obs) to give Structure Factor magnitudes. Calculating Structure factors F(calc) (and hence I(calc)) Calculating electron density using F(obs) and heavy atom phases. Phase problem in summing contributions from individual scattering factors Vector methods for overcoming the phase problem Agreement factors between data observed and calculated from the model Least-squares refinement to optimize this agreement
fundamentals and complete discussion of application to a specific project
incorporate structure into understanding of material science and nanotechnology, whether atomic or molecular structure
Same as undergraduate comments, except that one might envision more depth in a graduate level structural biology or biophysics course.
I would like to see a crystallographic computing class to teach the basics of programming and to teach a little bit about how various programs are really working i.e. what assumptions are they making and when are they valid.
Should begin with fundamental theory and be very thorough in both theory and application.
In a general course, it should include the basics of diffraction and Fourier constructions. It should also discuss the major problem (phasing) and how the problem is solved.
Symmetry, Diffraction, Phasing methods, Synchrotron methods, Density modification, Refinement, Model bias, Artifacts.
It depends on the area of concentration....from not much more than undergraduate to in depth understanding ...theory, application, etc
sufficient depth that the student can conduct an experiment themselves with some guidance & properly understand the results
As deep as possible

Medicinal chemistry
General knowledge of how to determine a structure beginning with a protein of interest For end users only: how to assess the quality of a structure and general concepts on how to interpret a structure [identifying motif/folds, active sites, binding sites, etc.] Students who specialize in crystallography/structural biology should pursue the advance topics of this field - mathematical basis/diffraction theory.
As in undergad. for students not intending to become crystallographers.
Probably a heavy emphasis on the quantum mechanics and physics, as well as possibly some computer-oriented computation.
The physics of diffraction and phase solution, symmetry, related methods (scanning probe, EM, theoretical modeling ...).
Item 8 plus: Lipson & Cochran, James, etc
space groups
prepare students for research
Considerable coverage of both powder-diffraction and single-crystal techniques and applications
A graduate course should be offered to be taken by geologists, physicists and chemists on X-ray crystallography.
In the earth sciences: relation between analytical data (from XRD, TEM, etc.) and crystallography of materials; relation between crystallography and crystal chemistry.
Students should be able to write computer codes to model X-ray diffraction patterns. Reitveld refinement should be taught.
Students should be able to write computer codes to model X-ray diffraction patterns. Reitveld refinement should be taught.
mineralogy, materials science
As needed for projects. Many projects require no crystallography at all, so those students don't really need it.
Much depends on the subtopics being studied. Again it should be taught to that depth necessary to avoid making bone-head mistakes for not recognizing the relevance of crystallography to the subject being worked on
Same topics as 8, with greater depth Techniques of crystal structure determination and physical property measurements
reciprocal space, structure refinements
materials science courses
Space groups.
varies by discipline
minimum of crystal systems, classes and symmetry operations so applications can be made to optical properties
Hands on lab experience in sample preparation techniques, data collection and analysis, and various structure methods (Fourier maps, etc.). Actually do it at least once to have an appreciation of what is required.
Heavy on crystal chemistry.
crystal structure understanding -elementary geometrical crystallography (lattice and parameter transformations) -Reciprocal space -crystallographic principles of the physical properties -crystal structure classifications
Some understanding of structure analysis

Symmetry, space groups, structures, physical properties (tensor analysis), elasticity
Same as undergrad, but in more detail
Instrumentation for XRD and neutron diffraction, methods of phase identification, quantitative analysis of mixtures, principles of crystal structure determination or refinement
Mathematical symmetry Space groups Instrumental techniques Structure solution and refinement
Through planes and lattices
Symmetry as far as space groups, XRD powder methods, systematic mineralogy, crystal chemistry
diffraction physics, group theory
Again heavy on the math with a focus on vectors, linear algebra, Fourier series, Fourier transforms, and tensors
Depends on objectives of graduate study. This might be covered as short 2 week courses
An advanced course on x-ray structure determination using single-crystal and powder methods.
symmetry, crystal growth theory, kinematic diffraction (mention dynamic), space groups, Fourier theory, structure solution, refinement theory, numerical and graphic presentation, reliability tests
Students should have an in-depth understanding of the link between crystal structure / defect structure and materials properties. Students should be able to examine a crystal structure and draw comparisons between that particular material and other similar materials. Students should be able to examine a crystal structure and identify coordination numbers of specific atoms, degree of polymerization (e.g., silicates). Students should understand epitaxic and topotactic solid-state relationships.
Moderate to completely mathematically rigorous treatment of theory of diffraction and analysis of diffraction results. Hands-on experience if at all possible.
Teach them how to solve and refine routine small-molecule crystal structures.
In-Depth coverage of diffraction methods and the results available from each. In-Depth course on single-crystal structure determination. In-Depth course on powder diffraction.
Bragg's law, scattering (elastic and inelastic), crystal space group symmetry, reciprocal lattice, Fourier transform

Respondents were asked to suggest specific courses where crystallography should be covered in the graduate *life sciences curriculum*:

An option to take a focused course is best.
Biology--perhaps in an instrumental course?
Biophysics, pharmaceutics, microbiology
specific course in biology dept.
structural biology
X-ray crystallography
No graduate students coming from biology, at present, will have had serious and competent instruction on 8. and 10. above.
Interpretation of results.
molecular biology, biochemistry, biotech
should offer a full course of diffraction theory and determination of protein structure by

nmr, spectroscopy, and crystallography
Same as above for physical sciences.
macromolecular crystallography
Medicine, pharmacology, etc. Graduate level biochemistry
Not at all.
Protein biochemistry. Nucleic acid biochemistry. Enzyme activity. Crystallography.
Biochemistry, Biophysics; stand-alone course: Crystallography
Practical protein crystallography
Biochemistry
general core class - advanced topics course
Biochemistry, Physical techniques in biochemistry, biological structure.
It should be taught in the research environment
Graduate Level Biochemistry. Biophysical Methods. Structural Biology. Macromolecular Crystallography.
Physical biochemistry, structural biology
In specialty courses.
Structural Biology
Briefly in biochemistry, should have a semester class devoted to it.
Biochemistry, molecular biology, cell biology.
Structural Biochemistry
Molecular Biology Protein Structures
Molecular biology
varies with curriculum
Ditto. Many in this field are very poorly prepared for this type of work. The result is some of the poorest quality "science" ever done.
application of XRD structural analysis of complex organic molecules
protein structure, enzymology, genetics, biophysics
I don't make a difference. Life sciences _are_ physical sciences (i.e. they are not Philosophy or Literature).
It should be a dedicated course.
For students entering a discipline in which crystallography plays an important role (molecular biology, molecular genetics), a thorough course on the application of diffraction to life sciences should be provided.
I use journal club/ seminar series focused on some topic in structural biology to introduce topics related to crystallography

Respondents then suggested the depth of coverage/topics that should be covered in crystallography in the *graduate life sciences curriculum*:

As much depth as possible in a one semester grad course.
Should be fairly in depth with the theory and should have some hands on experience built in.
The students should learn more about this topic, but I have found that few faculty outside of the biophysics groups have any interest or experience in crystallography.
Honestly, I'm not sure.
8. and 10. and 12. above. For potential practitioners direct methods, anomalous disper-

sion, synchrotrons, MIR and neutron diffraction are additional essential topics.
Enough depth so they will have an idea whether or not to trust results.
Fundamentals and complete discussion of application to a specific project. Both MR and Se-Met should be covered
at least one full time course for crystallography due to its prevalence in molecular biology, structural genomics, and pharmaceutical drug design
Same as above for physical sciences.
Can be a combined class with the physical science, we had two crystallography courses taught, one from the chemists which cover small molecule and some macromolecular and another taught by the biochem dept, which covered macromolecular. The biologist took both.
Focus should not be on theory other than a general understanding of the geometry of diffraction. Emphasis should be on understanding and using crystal structures, and understanding the reliability based on statistics.
Generally the technique and how solved.
Judging the quality of a crystal structure. Assessing its relevance.
It depends on the area of concentration....from not much more than undergraduate to in-depth understanding ...theory, application, etc
Goal for the general student should be to be able to read and assess a paper critically. What is involved in solving a structure, basic concepts such as resolution, R-factor, Free-R, data quality, model quality and model assessment.
sufficient depth that the student can conduct an experiment themselves with some guidance & properly understand the results
At least one semester, about 6-9 hours a week
The results in terms of protein structure are more important than the details of the methods.
General knowledge of how to determine a structure beginning with a protein of interest For end users only: how to assess the quality of a structure and general concepts on how to interpret a structure [identifying motif/folds, active sites, binding sites, etc.] Students who specialize in crystallography/structural biology should pursue the advance topics of this field - mathematical basis/diffraction theory.
As in undergad. For students not intending to become crystallographers.
Biochemistry: brief treatment--1 day or so. Biophysical Methods: major topic. Structural Biology: ~1/2 the course time. Macromolecular Crystallography: full-time in-depth.
More emphasis on the information from crystallography and how it integrates into other techniques to provide useful information. Some physics, quantum mechanics, and computer-oriented material should also be included.
How to benefit from structural genomics: how to find, explore, compare, and extrapolate from a model, and how structures can answer biological questions. The architecture of and inferred behavior of biological modules. Related methods for determining structural information.
I used to think every student should develop some critical sense and understanding of crystallographic papers. I'm not as optimistic now that that's an achievable goal. It's pretty easy to get students to be hypercritical, but most of what we do makes them unreasonably so. I suspect that the level of training needed to make them good critics would require many years of training and research in the field.
At the minimum, Blundell & Johnson's book

Enough to solve and understand macromolecular crystal structures

Biochemistry - usually there is limited time to cover any one topic, so just the basics should be covered Crystallography class - should cover all aspects to a moderate/advanced level

Visualization with more attention to the limitations and uncertainties in the data, including underrepresented categories (membrane proteins) and the importance of intrinsically unstructured proteins.

Considerable coverage of both powder-diffraction and single-crystal techniques and applications, particularly as applied to protein structure determination

Sufficiently deeply to avoid making stupid mistakes.

diffraction physics, point groups, space groups

Research dependent, I would say.

Methods of structure determination. Understanding the results of structure determinations.

Familiarity with Bragg's Law, resolution limit, R values, and capabilities and limitations of structural information obtained by crystallography

Respondents made the following comments with regard to hands-on laboratory training in crystallography:

It is useful to have students see the instrumentation and how it works. Perhaps show some axial rotation CCD frames But most can be demonstrated successfully with a computer.

Apart from math nerds, people can mainly be fascinated about crystallography when they see the output.

Yes it is essential. Without the hands-on training then the subject matter is to abstract.

Extremely important. More than textbook understanding.

Crystallography is difficult to get excited about as an abstract, classroom subject. There is a thrill in seeing 3-D views of new structures and examining atom connectivities that cannot brought alive in a classroom.

You need to bring the classroom topics alive with experience on the instrument and actually solving a data collection.

X-ray crystallography is such an important technique in scientific research that it should be a part of the graduate curriculum for all students involved in chemical synthesis, as is NMR, IR, etc.

This is how things are done.

Essential says it all. Anything less than hands-on training is short changing the students' experience.

If all a student does is tap keys on a computer, the essence of an experimental science is lost.

Anyone can memorize or have a slight understanding of the theory and physics behind crystallography, but its not until you actually see how it works that you can appreciate it.

Hands-on-lab encourages students who do not want to be xtallographers to solve their own structures as part of their own research interests.

Much of our work is in crystal engineering and inorganic chemistry, so we rely heavily on crystallography for structural solutions.

Crystallography is difficult to get excited about as an abstract, classroom subject. There is a thrill in seeing 3-D views of new structures and examining atom connectivities that

cannot brought alive in a classroom.
Essential for practitioners only. Important for users of data bases for powders and single crystal structures but their practical needs are different from working the instruments.
Crystallography needs hands-on laboratory to make sense!
Lecture without practical experience is much less useful than work including laboratory time.
Students don't clearly understand the concepts until put in practice. Laboratory includes using computational tools available.
Need to have some idea of what is involved, both in seeing what the experiment and interpretation is, and in understanding the literature.
It is essential only for those likely to want to do research requiring crystallography. The ideas and the ability to make intelligent use of the results are what others need, and that is sorely lacking.
Not every student, especially at the undergraduate level needs hands-on training, although this can enhance understanding at many levels. At minimum undergraduates should use molecular visualization tools to inspect macromolecular structures, and examine PDB files for quality.
Not everyone can be a crystallographer. However, the databases are proving more and more useful, and people emphasizing other areas need to know how to use the data created in other labs.
To know the molecules one is working with, a 3-D structure is invaluable. Modern equipment in crystallography makes it accessible to all.
Like NMR and many other techniques, for the most part, crystallography is a hands on practice and needs to be taught hands-on.
There is no better way to learn.
In my field - macromolecular crystallography - books will not teach you to be a good crystallographer. This is 100% an apprenticeship.
All real working crystallography was learned hands-on.
Again it is a function of area of concentration from not necessary to essential.
Important for chemists, inorganic chemists and physical chemists. Important for structural biologists. Not so important for general life science students.
Can't be properly done or understand otherwise.
Often class time is limited and therefore focused on the theory of crystallography - without practical application the theories are not grounded in a student's experience and therefore easily forgotten.
If you aren't going to do it you only need to see how it is done, not learn how to mount crystals, collect and reduce data etc.
For the courses Structural Biology and Macromolecular Crystallography, hands-on lab training in crystallography is essential. This is the only way to get a real feel for crystallography. While I would recommend wet-lab crystal growth, I don't see that as essential. However, data and phasing information should be available to work through the structure solution process. I see this as essential for really learning crystallography.
If someone wants to pursue crystallography, they must have lots of exposure during training. Because crystallography employs different skills at different stages, both wet lab and computational aspects are crucial.
Although essential to a potential crystallographer and important to a structural biologist, all that is needed for the others is hands-on experience with the products of structural

studies.
It's the way I learned it, and it's far better than just a bunch of lectures.
The ability to deduce space group from absences is a must. Understanding crystal symmetry, molecular symmetry, asymmetric unit, presence of half a molecule in the asymmetric unit, etc all these can come only through hands-on lab training.
We plan to do some protein engineering, which will require experimental validation. So far, we've focused mainly on structure prediction, for which one lab's experimental results are too few to have any significance.
It makes easy for the student to understand where the info comes from, and also makes them become more interested.
This should be available to grad students (or undergrad independent study students) who elect. Obviously this works only if there is at least one faculty member doing crystallography.
Thinking in 3 dimensions is easiest with 3 dimensional models, things that appear easy are deceptively difficult without hands on experience.
Essential, especially in beginning courses where students have not had prior exposure. Necessary to initially visualize what is going on.
It is useful but not essential for some students. The more hands-on the better they will appreciate this.
Hands-on experience is essential to understanding crystallography and appreciating its potential and applications.
It is not very important for undergrads in geology. It is important for graduate geologists who need to use XRD in their research.
Hands-on experience is crucial, particularly for studies of diffraction physics. Geometrical crystallography could be done without hands-on training, but it would be pretty dull.
No other way to learn it.
Analytical skills, machine techniques, procedure and processing, interpretation.
I see little likelihood that students (at least at the undergraduate level) will take much interest in this material if it is all taught at a theoretical level.
You've got to do it to understand it.
Theory is rarely sufficient to understand lattices, crystal structures and defects and such.
It's hard enough to think spatially with concrete hands-on examples & materials. It's almost impossible without.
Extremely important. Especially if one is to understand the physical properties of materials.
There must be balance here against the need for other needs.
Import for most physical sciences students; perhaps less so for life scientists specializing in organism level and above.
You can't learn this stuff entirely from a book.
It was very valuable to me as a graduate student and I still use things I learned in actually doing a structure refinement of a new mineral - I wish students around our department had the same opportunity.
These can be difficult concepts to grasp without working with real, three-dimensional objects.
Even for environmental science majors 3-D visualization is essential.
Because of the 3-D nature of crystallography it is necessary to do it to learn it. Reading

text or seeing diagrams in the book is not enough.
Far too much laboratory material is non-contact exercises, especially with "virtual" labs on CD's.
As equipment is becoming more expensive, it is tempting to keep students away and use dry labs, or canned labs. In the process (and through other societal changes) we have been raising a generation of students that do not understand how mechanical things work. We also have calls for more "experiential" learning. We should heed these calls.
Used as basis for interpretation of XRD patterns of minerals and synthetic materials.
My analogy will be the modern trend to teach principles of math rather than the solution of problems. That is baloney!! Knowing the principles of diffraction is not enough. If you haven't done it, then you are unable to realistically criticize the results and become totally dependent on statistical criteria that may be wrong. Just read some of the last works of Linus Pauling for a guide. He enjoyed showing that structures reported in the literature were wrong, but were statistically correct!!
Who do you know that understands XRD that hasn't actually run a pattern and tried to interpret it?
Trying to learn crystallography from a computer screen is a colossal waste of time. Models that the student can manipulate are essential.
For the most purposes the crystallography is just the necessary background of a method (there laboratory training is essential). However, there are also examples of a purely theoretical approach, where this is not very important.
Theory is no good without practical applications.
A basic understanding of crystalline solids does not require lab methods, but any involvement with experimental studies would require laboratory training.
It's essential to understanding optical properties of minerals and the use of petrographic thin sections.
Both laboratory and computer lab training is essential for truly understanding the underlying concepts.
Different instruments and software require hands-on experience to be useful, and for the theory to be converted to practice.
It's important for students to make the connection between the fundamentals (textbook & lecture) and real applications (lab work).
It's important for students to make the connection between the fundamentals (textbook & lecture) and real applications (lab work).
Definitely need models. The computer just isn't the same.
Undergraduates need the hands on to appreciate symmetry and how to identify it.
Very simple. I learn through my hands.
Hey you can get burned if you don't know what you are doing. Structure controls properties and function.
Hands-on laboratory training should go hand-in-hand with the theoretical aspects of crystallography for a thorough understanding of this interesting subject.
In my experience very little real knowledge is acquired without laboratory experience.
Research dependent, I would say.
Important for graduate students.
Important if the student is going to *do* crystallography, less so if the interest is only intellectual, but still worth while.

I don't do crystallography directly, at least right know, but sometimes I have to deal with phase transitions between different space groups and I don't always understand the differences between them.
Do not think people learn much without it.
I deal only with undergraduates, and have no way to give them hands-on experience. I try to help them understand the basics of the method and judging model quality (crystallographic, NMR, and theoretical models). I hope they will get hands-on experience in graduate school.
It depends on the number of students. If you can limit the number to less than 10, the students could gain a lot from hands-on-experience.
Otherwise it's meaningless!
It is as essential here as in any experimental science.
This depends very much on how the training will be used. For me it is essential, but for a molecular biologist or geneticist it may be sufficient to examine the concepts and leave the details alone.

Finally, the respondents were asked to make any additional comments:

You might wish to ask about necessary reference materials.
With very few exceptions, academic institutions typically do not hire crystallographers. They hire chemists or biochemists who know something about solving crystal structures. I think this is a grave mistake.
Crystallography is the best way to introduce more about the solid state into the curriculum. Several recent workshops have emphasized solid-state areas for future research in chemistry. Our students spend far too little time working in areas where chemistry is headed.
The lack of texts at the appropriate level is very limiting. Too many teach Fourier theory and other topics students will not use or can look up and not enough of what actually takes place in a typical experiment.
Modern chemistry and physics professors have scant training in these concepts and will begrudge undergraduate teaching time even for very basic material. Inorganic people are far easier to persuade than organic or life science teachers; even if you smack them in the eyes with their own journals!! It is possible to sneak these concepts into courses which are labeled "inorganic and organic solid state structures" If the word "solid" isn't in there the local organic nmr expert will volunteer to teach the course even though his own supreme technique already has lots of teaching time.
It is important in a graduate education to understand and evaluate the literature, and this includes understanding and evaluating the results of a protein structure, relation to the function (kinetics), thermodynamics of binding ligands, computational aspects of ligand binding, etc.
In view of the fact that experimental structure determinations will never be available for all proteins of interest, increasing attention to homology modeling becomes necessary. This has driven our work in curriculum development and should be the province of the 3D structural community.
Considering X-ray crystallography is a linchpin of understanding of protein function, it is actually astounding it gets so little coverage in most undergraduate curricula. Part of the problem is that most faculty are not exposed to this field either, and cannot be expected to be effective teachers for their students in this regard.
Students need to be more than button pushers.

Post-graduate education is also sorely lacking in North America, cf. European "short-courses" which are regularly held throughout the EU.
The Education Committee of the US National Committee for Crystallography should set up an all-encompassing online course available to those interested in following a rigorous curriculum.
Much of the training at the graduate level for crystallographers takes place at courses held once per year at places like CSHL and BNL. The courses are high quality, as they bring excellent instructors from all over to teach.
At the undergraduate level, at least one small molecule structure should be solved, in physical science as well as life science stream.
Your classification into life sciences/physical sciences is too crude to be meaningful. Your focus on crystallography as the only experimental method for determining molecular structure is also rather limited---NMR has also a major role to play.
Does the USNCC have a website? What about it's Education Committee? If so, I hope they will provide links to Protein Explorer, http://proteinexplorer.org (Trends Biochem Sci, Feb 2002, 27:107-9.) It is the easiest macromolecular visualization tool and also a knowledge base with links to key external resources such as EBI's Probable Quaternary Structure and Tel-Aviv's ConSurf evolution display server. Protein Explorer was designed for students and educators but has also been used by researchers. Its main page is visited 3,000 times/week and although it can be used very effectively on-line, it is downloaded 40 times/day. -Eric Martz, Univ. Mass. Amherst.
This survey is restricted to physical and life sciences, but misses the importance of chemical sciences (at all levels). Also, it misses the graduate level importance of the geological and materials sciences.
Crystallography is the basis of crystalline materials in the earth - too much is being left out of undergraduate mineralogy courses with the concept that teaching crystallography is old fashioned and not useful.
With the current emphasis on more "meaningful offerings at the undergraduate level" courses such as crystallography or even its incorporation at a greater level in geology curriculum is doubtful. Time constraints, equipment, maintenance of machinery (I teach the course, I run the machine, I troubleshoot the machine, I program the computer software, etc. - no tech support) are all major considerations and with the tight budget at this university (and others), as well as the issue of course load and "relevance" the potential for adding a more complex course (or topic area) may not be deemed "cost effective".
If there isn't improvement here with respect to general awareness of the relevance of crystallography to the other sciences, a lot of damage will be caused the scientific research in general.
You didn't ask about the general level of science training of the undergraduate population. It is either poor or nonexistent at many institutions.
As a geologist, I am aware that virtually all of the material that I deal with is crystalline, and how it interacts with ground water, in a porphyry copper milling or leaching system, with a melt, in a diagenetic sandstone, in a fossil mammal bone, in a deforming fold, or hydrothermal vein, is controlled by properties at the level of the unit cell. I want to hire people who understand, and can use that information even though "crystallography" is not part of their job description.
An introductory course in mineralogy of materials, taught from an interdisciplinary approach, could provide basic crystallographic considerations and other principles common to physical and biological sciences.

My experience in working with modern material scientists and medical doctors is there total lack of preparation in critical areas of crystallography. Some can talk a good game, but have never played. Geology is no better. Some departments have replaced traditional courses in mineralogy and crystallography with some baloney called "earth materials." Why?? Because traditional courses were too hard for many of today's soft-headed, spoon-fed students at both the undergrad and grad level. The recent disclosures of the Crick and Watson in stealing the data to determine the structure of DNA (they couldn't generate it because they didn't know how) clearly indicates the state of concern regarding crystallography that started to decline in the 1950s and 1960s. Computers and statistics are not replacements for thinking and understanding.

It would help if the vocabulary used in the different disciplines were more uniform. For example, I like the analogy that structure (as in crystal structure) is to the brain as lattice is to the mind. However, there doesn't seem to be a general recognition of the distinction between structure and lattice.

Crystallography is probably the best subject to teach spatial relationships to students. This is very important and they won't get it elsewhere.

Mineralogy, the context for crystallography in the Earth Sciences, remains an important component of undergraduate training, although it has been diluted to varying degrees by the need for other courses in environmental geology and geochemistry. Crystallography per se is done by fewer institutions, although there are some centers of excellence such as SUNY Stony Brook, Carnegie Institution, that do crystallography.

Maybe short courses are the answer. We can't teach everybody everything but we can teach how to approach problems and we should have some teaching aids and methodology available for those who have interest and needs in this area.