

19-Crystallographic Teaching and the History of Crystallography

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OCM-19.01.04

TEACHING THE ELEMENTS OF DIRECT METHODS by Henk Schenk*, Laboratory for Crystallography, University of Amsterdam, Nieuwe Achtergracht 166, 1018 WV Amsterdam, The Netherlands.

In a diffraction experiment intensities I_{hkl} are measured whereas $F_{hkl} = |F_{hkl}| \exp(i\varphi_{hkl})$ are necessary to image the electron density. Now $|F_{hkl}|$ can be calculated straightforward from I_{hkl} but the relative phases φ_{hkl} are lost in the experiment and cause the so called phase problem. Direct methods try to evaluate phases φ_{hkl} "directly" from the measured diffraction intensities I_{hkl} by using relationships among the phases, relationships, whose values are based on the intensities only. Roughly it can be stated that, since the crystal structure can be described by a limited number of parameters (the positions of the atoms) and since many more intensities can be measured, relationships among the structure factors F_{hkl} , and thus among the phases φ_{hkl} , must exist. Direct Methods identify and use these phase relationships to solve the phase problem. In a nutshell a Direct Method proceeds as follows: In the first step as many phase relationships as possible are collected, the origin is fixed by specifying the phases of a few suitable reflections numerically and then, using the phase relationships, new phases are calculated. In general, however, it will not be possible to phase all strong reflections and hence a few more starting reflections are selected, which act as unknowns (symbols, ambiguities) and from which new phases can be calculated using the phase relationships (the so-called phase extension). This process generally develops like a snow ball, provided a good choice of origin-defining reflections and unknowns has been made. Finally, when most of the strong reflections have got a phase, the numerical values of the unknowns are evaluated and using a Fourier summation (expression 1) an image of the structure is produced.

Teaching of Direct Methods should focus on the explanation of the relationships and the use of these relations in actual phase determinations. The author will show some of the material he uses at the University of Amsterdam based on the physical meaning of triplet and quartet phase-relations. It includes an introduction to a CAI on Symbolic Addition, to be presented as poster (Y-F. Wang).

OCM-19.01.05 PHASES FOR PROTEINS. By Wayne A. Hendrickson, Howard Hughes Medical Institute, Department of Biochemistry and Molecular Biophysics, Columbia University, New York, New York 10032 USA.

While the phase problem in macromolecular crystallography is in essence the same as for small molecules, its solution in practice is typically quite different. As these structures are too large to be solved by conventional direct methods or by Patterson techniques, heavy-atom labels are used to reduce the initial problem to one of manageable size. Thus, the methods of multiple isomorphous replacement (MIR) and multiwavelength anomalous diffraction (MAD) make possible the *ab initio* phase evaluation for protein structures. Powerful methods have also been devised for refining initial phases by molecular averaging, solvent flattening or other electron-density modifications. Many interesting macromolecular crystal structures have analogous counterparts in the database of known protein and nucleic-acid structures, and these can be analyzed by the methods of molecular replacement.

Although the armory of techniques for macromolecular phase determination are becoming increasingly automated, the need remains to teach new practitioners the basic elements of both experimental design and computational analysis. Moreover, as teachers we hope to stimulate some students to advance the methods in this exciting area.

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TEACHING THE RELATIONSHIP BETWEEN THE X-RAY DIFFRACTION PATTERN AND THE ELECTRON-DENSITY MAP: FOURIER SERIES AND TRANSFORMS. Jenny P. Glusker, The Institute for Cancer Research, 7701 Burholme Avenue, Philadelphia, PA 19111, USA.

The teaching of structure determination by diffraction techniques will often give very little time to the relationship between the diffraction pattern and the electron density map. The significance of this relationship in terms of Fourier series will be discussed. The Fourier transform can be taught at various levels, but the simplest relationship is that described by J.M. Bijvoet in his book *X-ray Analysis of Crystals*. In this he considers the effects of very simple electron density profiles. The student will need to become thoroughly conversant with the Fourier transform in order to appreciate the power and limitations of X-ray diffraction as a method of crystal structure determination. Some simple cases that can be used as teaching aids, particularly to students who do not like mathematics, will be presented.

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THE IUCr TEACHING COMMISSION PAMPHLET PROJECT. Jenny P. Glusker, The Institute for Cancer Research, 7701 Burholme Avenue, Philadelphia, PA 19111, USA.

The pamphlet series of the IUCr Teaching Commission was organized by Dr. Charles Taylor when Chairman of the Commission. These pamphlets are available from Polycrystal Book Service. This project is now being reinstated and several submissions are now under review.

PS-19.01.08 STRUCTURE, CRYSTALLOGRAPHY, & DIFFRACTION in the TEACHING of CHEMISTRY with EMPHASIS on ORGANIC & BIOCHEMISTRY at a TWO YEAR COLLEGE by BRAHAMA D. SHARMA Chemistry Departments, Cal State Univ. L.A., Los Angeles, 90032 & L.A. Pierce College, Woodland Hills, CA 91371 USA.

The importance of relation of structure to function or function to structure (including dynamics) is pivotal to the TEACHING of chemistry. Specific examples will include (1) how in health related & biochemistry courses the stereo-specificity is fundamental. The absolute configuration is made possible by DIFFRACTION using the anomalous dispersion.

(2) how in general chemistry the choice of thermodynamic standard is based upon the crystal structure as in diamond & graphite- A SURPRISE IN THAT thermodynamics is not supposed to be based on structure.

(3) how in general chemistry one need to be cautious that two or more crystalline forms of a substance are not really polymorphs as will be shown for empirical formula EN solids.

(4) how in Diels-Alders reaction one needsto pay attention to structural dimensions of DIENE & the DIENOPHILE to see that the usual presentation of the desired product need§ re-evaluation.

(5) how function of a compound by LOCK-KEY mechanism may involve more than one LOCK-KEY pairs for the same parent compound as in PHENOTHIAZINES.

(6) how in Quantitative course the quantitative determination one needs to know the crystal structure to take a specific method as a means of determination as in FAJAN's method of determining chloride.