19.2–2 BASIC CRYSTALLOGRAPHY FOR CELL BIOLOGISTS. By R.H. Lange, Department of Anatomy and Cell Biology, University of Giessen, Aulweg 123, D-6300 Giessen.

Although structure research has recently been made more public among biologists in general (Nobel Prize to A. Klug), it is still little appreciated (textbooks!), its University representation is poor, and understanding of its basis is lacking in biology and medicine. As a consequence, a great number of, e.g., natural crystalline aggregates, continue to be published without adequate analysis and thereby escape utilization in the important task of rebuilding the "ultrastructural" at the structural level. Basic crystallography is, reasonably indeed, to be considered as a must in cell-biological training. In the sense used here, it includes the crystallographic way of thinking as required for treating ideal biomacromolecular crystals, simple geometrical and computational means for describing such crystals and the special use of the prime instrument of cell biologists, the electron microscope, for the study of biomacromolecular crystals. We thus focus on understanding and not on highly instrumentalized and computerized specialties, which, in fact, can produce erroneous results if performed without such understanding. There being no basic crystallography without crystallography, such a program has the following structure (arranged according to didactic needs):
1. Crystal geometry. Symmetry elements. One-, two-, three-dimensional translational lattices and their geometrical symmetry; conventions as to settings; stereographic projection; symmetry of projections; reciprocal lattice.
2. The biomacromolecule and its symmetry. Actual biomacromolecular symmetric structures; selected point symmetry groups; line symmetry groups; one-, two-, three-dimensional space groups; correspondence between lattice and structure symmetry; pseudosymmetry; quasi-symmetry; local axes. (Bernal in: Wolstenholme and O'Connor, Eds., Principles of biomolecular organization, p. 1, London 1966; Klug in: Engström and Strandberg, Eds., Symmetry and function at the molecular level, pp. 425, Stockholm 1969; Matthews and Bernhard, Ann. Rev. Biophys. Bioeng. (1973) 2, 257; Klug, Crick and Wyckoff, Acta cryst. (1958) 11, 199; Holser, Zschr. Kristallogr. (1958) 110, 266; Int. Tables X-Ray Crystallogr. I; Caspar and Klug, Cold Spring Harbor Symp. Quant. Biol. (1962) 27, 1).
3. Diffraction; amplitude and phase; X-ray and electron single-crystal and powder patterns; Ewald's sphere; reciprocal space; phase problem; Fourier syntheses.
4. The electron microscope as instrument in biomacromolecular crystallography; specimen processing; the goniometer; electron diffraction; calibration; causes for inaccuracy of the EM approach; electron imaging; optical diffraction; data handling and processing.
5. Practical problem: estimation of lattice parameters and discussion of apparent symmetry of an unknown specimen by electron microscopy.
Such a training program has been implemented in various abridged versions for interested students during a class requiring at least 20 hours (without practical problem), the limitation to enantiomorphic symmetry groups leading to a considerable reduction of matter.
Epilogue: Due to the severe limitation of electron microscopic resolution (2 nm) in typical biological specimens, all electron microscopic estimates of symmetry at the molecular level, on the one hand, necessarily remain provisional. On the other hand, the bio-medical electron microscopist does the pre-screening of biostructures; he should be enabled to do so and to predict what may show up once his specimen has passed an analytical procedure at higher resolution; due to the enormous problems of structure research in biomacromolecules, taking advantage of so much a-priori knowledge, as is offered by crystallography in apparently crystalline specimens, is of great importance.

19.2–3 A ONE-AXIS FLIGHT-TIME NEUTRON SPECTROMETER FOR STUDENT USE. By C. G. Shull and A. Zeilinger, Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, U.S.A.

A very simple neutron beam chopper has been used for many years in student experimentation at M.I.T. to examine the thermal spectrum of neutrons from a small reactor. When coupled with a crystal spectrometer, Bragg diffraction peaks may be easily observed in the flight time spectrum as displayed in a multi-channel-analyzer print-out. The chopper is a cadmium disk of diameter 11cm with eight radial slots so that rotation produces periodic neutron bursts, normally of frequency 250/sec with FWHM 100μs. A small optical photodiode whose output is also interrupted by the slots is used to establish the origin time of the neutron burst. Flight distances of 2m are normally used and neutron detection is made with a small, high pressure He^3 counter. The system has been used for various student experiments, including (a) full spectrum and neutron temperature determination, (b) establishment of Bragg diffraction from various crystal planes, (c) quantitative test of the DeBroglie relation, (d) transmission cross section measurements of various materials including the v^{-1} variation in absorbing boron, and (e) monochromatic beam depletion in the spectrum passed through a crystal. These experiments are routinely done within the Junior physics laboratory course at M.I.T.

19.2–4 PRINCIPLES INVOVLED IN THE DEVELOPMENT OF EXPERT SYSTEMS FOR DATA ACQUISITION H.J.Milledge (Crystallography Unit, Geology Dept.) C.M.O'Brien (Statistical Science) & G.I.Webb, University College London, Gower Street, London WC1E 6BT, U.K.

Although many thousands of crystal structures have now been determined, crystallographers have been relatively slow in accepting the validity of least squares refinements "constrained" by chemical information already available, though most now do so.

Procedures for incorporating chemical information into least-squares refinements which were described (I.U.Cr. Abstract 23.1-2, 1975) and which involved various assumptions concerning the ways in which heterogeneous data sets should be combined, can also lead to to the development of "expert systems" of data acquisition.

Such systems are particularly relevant to diffractometer data, which are now usually collected in a routine manner unrelated to the characteristics of the data set involved, although the time taken to measure a single reflexion and its background, perhaps of the order of a minute, gives the associated computer controlling the data acquisition ample time to update its current information and modify its future activities.

An attempt is made here to illustrate the basic principles involved in the design of such an "expert system" in the hope that future generations of crystallographers may come to regard "routine" data collection as having the the same relative efficiency as "unconstrained" least-squares refinements.