

19.X-7 THE CHESTER COMPUTER AND THE IUCr JOURNALS. By D.W. Penfold, Technical Editor and Computer Manager, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

A computer system, based on a Z80A microprocessor, with cartridge disc (15 MByte), cartridge tape back-up, six terminals and two printers has been installed in the Chester office of the IUCr. Its main uses are to handle the accounts of the Union and the journal production records for *Acta Crystallographica* and *Journal of Applied Crystallography*, to check for submission of duplicate structures and for resubmission of papers rejected by other Co-editors, and to produce the indexes for the journals. It is expected that both annual and quinquennial indexes will be produced far more quickly than with traditional methods and at a much lower cost to the Union. An investigation is also being carried out as to whether it will be feasible to take the checking of crystal structures a stage further by interacting with the existing crystallographic data bases. Programs have been specially written (in Basic) to carry out the above functions and the system is menu-driven so that much of the work can be done with minimal training. The indexing and duplication detection routines will be described and possible further future applications considered.

19.X-8 WRITING BETTER PAPERS. By G.A. Jeffrey, Dept. of Crystallography, University of Pittsburgh, Pittsburgh, PA 15260 U.S.A.

Two basic rules: for authors, present original work free from errors; for editors, make no changes without authors permission.

Acta A and B. Avoid the laboratory notebook, chronological or stream of consciousness styles. State the objectives and the degree to which they are achieved at the beginning of the paper, then give the details of the theory or experiment, necessary to support the conclusions. Do not write a detective story. Put the conclusion at the beginning of the paper, not at the end. As far as is possible use small standard words. Do not invent new words.

The sentence structure should emulate the style of early Hemingway rather than late Henry James. At the end of the writing, scrutinize every word and remove if not necessary. Remove or replace any words which do not have a precise meaning.

Acta C. These are depositions of crystal structure data, rather than scientific papers. Editors and referees require the full experimental data to verify the conclusions, but I question the necessity to publish them. I favor abstracts only, with concurrent entries into the appropriate Crystallographic Data File. This would advance the access by computer to these data by twelve months.

19.X-9 THE ROLE OF CRYSTALLOGRAPHY IN ELEMENTARY SCIENTIFIC STUDIES. By A. Guinier, Laboratoire de Physique des Solides, Orsay, France.

The majority of the students in science will never become specialists in crystallography. But many will need some notions of atomic structure of matter in their professional life. What will be useful is not the elements of crystallography, but important results, sometimes quite recent.

A course, adequate for non-specialists, is necessarily short; it cannot be neither a summary nor simply the beginning of a traditional crystallography course. One must abandon a strictly deductive approach; some fundamental ideas are presented without demonstration; many too specialised chapters of usual text-books must be suppressed but the implications of the crystallographic models in various techniques or sciences may be more developed.

For the beginners, two points are essential: the atomic radii or the covalent bonds and the separation between disordered and ordered states of matter. What is important is not the description of various types of order but the consequences of order upon the physical properties.

For future physicists, the concept of symmetry which appears in so many domains, may well be explained with crystallographic examples. For material science, the more important point is the understanding of the crystal-line defects and of their role.

Such courses, although elementary, demand a great effort to the professor. If he has been educated as a crystallographer, he must avoid to be too specialised, and if he is not, he has to extract what is essential from too complicated books: in fact, few books have been written to help him in this difficult task.

19.X-10 TEACHING CRYSTALLOGRAPHY FOR THE EARTH SCIENCES AND FOR CHEMISTRY. By Th. Hahn, Institut für Kristallographie der RWTH, 5100 Aachen, FRG.

Not only in research but even more in teaching, crystallography is a strongly interdisciplinary science. Usually only a fraction of the teaching activity of a crystallographer is devoted to future crystallographers, the larger part being addressed to students of other fields. In this lecture the needs of earth scientists (mineralogists, geologists) and chemists will be discussed.

Basis of all crystallographic teaching is the concept of periodicity, symmetry, and groups, i.e. lattices, point groups, space groups, and their applications to crystal structures. These topics require assisted practical exercises to be comprehensible.

Equally important for more advanced chemists and mineralogists are diffraction methods and elements of structure determination. Powder methods and their use are a 'must'. Film cameras help the student to understand the reciprocal lattice, automatic diffractometers educate 'black-box' mentalities.

There appears to be a danger, however, that crystallographers stop their teaching at this point and leave the treatment of the results of these methods, i.e. crystal chemistry and crystal physics, to other scientists. It is most important that the foundations (not the specialties) of these fields also are taught by crystallographers: Chemical bonding in crystals, ionic-covalent-metallic radii, coordination polyhedra and their connection, order-disorder, polymorphism, solid solutions, defects, etc., always demonstrated on actual crystal structures of elements, simple compounds, silicates, etc. The anisotropy of physical properties has to be brought out especially.

A survey of all these topics can be achieved in a one-semester introductory course on crystallography.