19.X-14 CLASSICAL TYPES OF PRINTED INFORMATION SOURCES

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Information sources are of two broad types, those intended for current awareness (publications up to,say, five years old), and those intended for retrieval (from, say, the beginning of the subject up to, ideally, a year old). There is, obviously, a considerable overlap. For current awareness in crystallography the most convenient source is the section *Cristallographie* of the *Bulletin Signalétique*. *Chemical Abstracts* contains more informative abstracts, but is very bulky.

For single-crystal data *Strukturbericht* and its continuation *Structure Reports* are the most informative sources, and often the only ones complete enough to avoid the necessity of consulting the original publication. For powder data the various files and indexes published by the International Centre for Diffraction Data (JCPDS) are without a rival. The series *Molecular Structures and Dimensions* give easy access to bibliographic information on organic and organometallic substances, but for numerical data it is necessary to go to the original publications or computer tapes. Similar projects for metals and inorganic substances are less advanced, though Pearson's *A Handbook of Lattice Spacings and Structures of Metals and Alloys* is a good source up to a year or two before its date of publication. Convenient sources of restricted types of data are *The Barker Index of Crystals*, *Crystal Data*, and some others.

Some early sources, now mainly of historical interest, will be discussed because of their influence on the development of current sources. Sources requiring the use of computers are treated at length elsewhere in this Congress.

19.X-15 SOME EXPERIENCES WITH COMPUTERIZED INFORMATION SYSTEMS. By W. B. Schweizer. Laboratorium für Organische Chemie, ETH-Zentrum, CH-8092 Zürich, Switzerland.

Computerized data retrieval is becoming an increasingly important technique for scientists. Files of crystal structure data now exist for proteins, organic and inorganic compounds; powder diffraction data files are also available.

There are two types of data files: sequential files, mostly used in non-interactive systems (batch mode), and inverted files for interactive systems. Interactive systems require only minimal computer knowledge. They are therefore suitable for data centres that work on a worldwide basis through computer networks. Because of the prompt response, mistakes and inefficient search strategies are detected immediately. This method is very powerful for retrieval of literature citations. Computer-drawn pictures of molecules can also be obtained very easily, together with their interatomic distances and angles. For searches of complex molecules or fragments, and even more for special geometrical calculations and statistics the interactive systems are often not flexible enough, because the data are encoded in a special way designed to handle specific questions. It is easier to modify programmes that use a sequential file where the data are not specially coded. The disadvantage is that searches on sequential files are normally more time-consuming and require different search strategies. With an interactive system one should start with global questions and restrict the number of hits by intersecting files, whereas a search question on a sequential file should give a useful answer in a single run if possible.

The user of a data file expects complete and up-to-date literature references. It is also important that relevant data omitted from printed publications should be available from such files.

19.4-01 THE ROLE OF A MICRO-COMPUTER IN A PROGRAMMED COURSE IN CRYSTALLOGRAPHY FOR UNDERGRADUATE CHEMISTRY STUDENTS. By A. van der Voort , B.F.K. van Santen, J.Jurriaans and H.Schenk, Laboratory for Crystallography, University of Amsterdam, Nieuwe Achtergracht 166, 1018 WV Amsterdam, The Netherlands.

In our department crystallography is taught to undergraduate chemistry students by a programmed instruction course. The average student completes the course in about three weeks of 35 working hours, in which (s)he is introduced to crystals and their geometry, X-rays, X-ray diffraction and applications of X-ray diffraction such as crystal structure determinations, identification of materials by powder diagrams. The course was written in Dutch by more than 10 authors, all of them students, coworkers or former coworkers of our laboratory.
In this paper we describe the latest developments, which were enabled by the availability of low-cost microcomputers. For our purposes we acquired a micro with low-resolution graphic facilities (TRS 80). In the section on Fourier theory and its application the micro is used to perform a one-dimensional Fourier summation of NH_4HgCl_3. The summation is evaluated interactively and calculated term by term at an interval of 0.02 along Z. The results are visualized at the CRT-monitor. The section on Direct Methods was upgraded by a triplet search program, and an interactive symbolic-addition program. In the latter, the student makes the decisions and the computer does the administration. A new section is the one on model building, starting from the results of a structural paper. The co-ordinates and unit-cell constants are used to generate interactively newman projections which are then used by the students to construct a Framework Molecular Model.
Finally, a new block provides instruction on the isomorphous replacement method starting from difference Patterson functions.