Consequently, the IUCr commissioned a working group to extend the CIF definitions to cover the macromolecular case. The members of the working group are Drs. Paula Fitzgerald (Chair), Enrique Abola, Halen Berman, Philip Bourne, Eleanor Dodson, Arthur Olson, Wolfgang Steigemann, Lynn Ten Eyck and Keith Watenpaugh. This working group is presenting this macromolecular extension of the core dictionary to the IUCr for formal approval at the 1993 Congress in Beijing. Following the recommendations of its executive advisory board, the Protein Data Bank will be adopting CIF as the new format for the crystallographic information distributed by the PDB.

The working group is actively seeking input from the crystallographic community concerning the macromolecular CIF dictionary. The completeness and accuracy of the definitions along with the completeness and clarity of the accompanying documentation is an ongoing project.

OCM-18.02.08 THE CIF DDL DICTIONARY AND ITS ROLE IN CIF SOFTWARE APPLICATIONS By S. E. Hall, Crystallography Centre, University of Western Australia, Nedlands 6009, Australia.

The Crystallographic Information File (CIF) was adopted by the IUCr in 1985 as a primary method for exchanging data and information between crystallographers electronically. This approach has proved successful and, with the widespread availability of CIF and its software in the crystallographic community, it is now being used by a variety of applications for exchanging data and information. The CCDC (Cambridge), JCD (Manchester) and PDB (Brookhaven) databases are expected to adopt CIF as their preferred data exchange medium. Other major data bases will follow, especially when the check CIF data become available directly from the CIF archives in Chester.

The existence of precise data definitions in the form of the CIF dictionary has been essential in the widespread acceptance of the CIF approach. The first electronic CIF version of CIF was released in 1991 as 'cif2c94'. This contained the definitions of data elements commonly used in small molecule studies. At this conference the definitions of powder and macromolecular data, coordinated by working groups headed by Brian Toby and Paula Fitzgerald respectively, will be presented for ratification by the IUCr CIF Committee. Following this, the CIF dictionary files 'cif2p93' and 'cif2m93' will be released for applications in these fields.

This talk will highlight the properties of the DDL CIF dictionary and how it is applied by computer programs such as CYCLOPS, CIF/EXS, and Star_Base. It will describe how CIF applications can be made and highlights some of the problems arising from their organisation and technology.

18.03 - Electronic Diffusion of Information

DS-18.03.01 COMPUTER NETWORKS: THEIR USE AND LIMITATIONS By Y. Ebelin, Laboratoire de Mineralogie-Crystallographie, URA 079 CNRS, Universit'es P.M. Curie et Paris VII, 75252 Paris Cedex 05, France

The establishment of a computerized World Directory which is now underway has lead to a general thinking about the use of networks in information exchanges between scientists. In this talk we will describe how the networks can be used and the limitations arising from their topology and technology.

The most widely used technology, nowadays, is an extension of the local area network protocol TCP/IP better known (but improperly) as Ethernet networking. Its development is linked to the diffusion of Unix. The second one is an IBM technology used in the famous Internet network. ISO protocols such as X.25 have been installed in United Kingdom (Janet) and are developing in other European countries. In other communities such as astronomy (SPAN) a digital technology is used everywhere. This diversity restricts the exchanges between the different networks. Electronic mail is the only flow of data which circulates easily between networks and other information (software, data) are often encapsulated in messages which severely restricts the possibilities of communication.

However, more and more people have a transparent link to the TCP/IP world which allows various communications which will be discussed in this talk:
- e-mails which pass through all networks and which may be used to address a query to a server. The world directory will be available to everyone by this means, sending queries in messages and receiving the answers from the server in the same manner.
- lists where people are registered on a list and receive all the information, moderated or not, which is addressed as messages to the list. The use of lists is compatible through different networks.
- bulletin boards where people establish a connection to a server and consult a given information menu by menu. It is restricted to the feasibility of establishing a connection to the server and retrieving a piece of data. The restrictions are the same as for bulletin boards. Scientists will have access to the World Wide Web by this means.
- anonymous ftp, mainly restricted to the TCP/IP world, which allow to retrieve character and binary files.

A new technique is developing, based on a client-server protocol where part of the software is resident on the user's machine, part on the server.

Other limitations appear when exchanging formatted documents which contain text, formulae and drawings. However one may foresee the day when the IUCr Newsletter will be available through the network.

The advantages, possibilities and limitations in the use of networks will be discussed explaining the choices for the World Directory of Crystallographers.

DS-18.03.02 DISTRIBUTED NETWORK INFORMATION SERVERS By B. McMahon, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England

It is almost commonplace in the modern world that valuable and useful data may be accessed and retrieved from databases, file transfer archives and electronic bulletin boards. Crystallographic structural data are now archived on the IUCr Editorial computer system, thus making feasible the concept of an electronic journal of crystallography. The logical extension of these ideas is the provision of an electronic library, a facility for retrieving diverse information from any of a collection of sites providing data.

Already, the use of standard protocols across the global Internet has given rise to several tools for viewing the library resources of various archive sites, such as oasis, gopher, it is available at the University of Minnesota, provides a hierarchy of menus allowing direct access to data categories. Each entry in the menu may represent data stored on a machine, anywhere in the world. The casual user may choose a menu item without knowing or needing to know the location of the information sought.

The WAIS (Wide-Area Information Server) system is a standard way of indexing the textual content of files stored at an archive site. A WAIS request can select from a document collection all files containing a requested word or term. It can rank the selected files in order of likely relevance by applying a heuristic test based on the number of occurrences of the target term, and in principle possible to perform searches based on context. WAIS is often used to supply index services to a data collection initially accessed through gopher.

A third global information dissemination system, WWW (World Wide Web), developed at CERN, provides formatted documents to be read on-screen at the user's convenience. Hypertext links within the document allow cross-references to be followed as the document is perused. As with other tools, the links in the hypertext chain may reside on physically remote computers.


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