possible errors in the input data. A systematic survey of structures in the Inorganic Crystal Structure Database shows that the program can provide a proper description of the chemical bonding for about 90% of the error-free entries and in 67% of these cases it can recognize that it has been successful. The output of this program is a listing of all the bonds formed by each cation and includes the bond length and valence, the bond vector and the symmetry transformation applied to the terminal atom (anion). This file is being used in the first instance to produce a bond index similar to that in BIDICS and later will be used to construct a connectivity index that can be searched by computer. Problems arise in constructing a connectivity index of inorganic solids from two sources - the continuous range of bond strengths present and the existence of networks with crystallographic translational symmetry. The former can be treated by allowing the user to define a threshold bond valence below which the bonding network is ignored. The latter requires careful treatment of the crystallographic symmetry by the computer so that the user can manipulate the structure without having to worry about space group operators and special positions.

These ideas can be extended to the predications of crystal structures. We have so far developed algorithms which successfully predict the chemical bonding network and bond lengths in most ternary compounds using only a knowledge of the coordination numbers and oxidation states of the constituent atoms. We hope to be able to solve the more complex problem of mapping the chemical bond network into the crystallographic bonding network once we have developed a proper description for the chemical connectivity in terms of the lattice symmetry.

19.1–4 STORING OF DATA OF OD-(ORDER-DISORDER) SUBSTANCES. By K.-O. Backhaus, H. Grell, Zentralinstitut für physikalische Chemie & H. Schrauber, Zentrum für Rechentechnik, Akademie der Wissenschaften der DDR, Berlin.

Besides the bibliographic file, OD specific data are stored. These are: The OD groupoid family with the net constants of the layers and parameters of the layer pairs. In detail are given: Atomic coordinates of atoms belonging to one OD layer, transformation matrices of the layer group and of the space transformations transforming one layer into the next layer. With this information deducing of any stacking of layers is possible, especially that of MDO structures or of periodic structures of any length. Simulated diffraction patterns allow comparison with the x-ray image of actually occurring substances.

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19.1–3 CURRENT DEVELOPMENTS IN THE CAMBRIDGE STRUCTURAL DATABASE. By Olga Kennard, F.H.Allen, Sharon Bellard, J.E.Davies, J.Galloy, R.F.McMeeking, R.Taylor & D.G.Watson. Crystallographic Data Centre, University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, England.

By 1st Feb. 1984 11,670 new entries had been added to CSD since the Ottawa Congress. The total database (41,725 entries) is now available in 25 countries. Additionally a number of major system developments are nearly complete :

Chemical Graphics. Programs have been developed to input, edit,store and display chemical structural diagrams. The current input is digitized via a Tektronix minicomputer; connectivity records are generated which contain 2D (x,y)-coordinates for each atom. Over 13,000 diagrams have now been input and published in Vols. 13-15 of MSD.To upgrade the backlog a program has been written to generate (x,y)-coordinates directly from the existing connection tables.

Integrated File Structure. The previously separate files of bibliographic, connectivity and numeric data have now been amalgamated into a single internal archive file. This complex undertaking required a major upgrade of CCDC internal software. Work is now directed towards a flexible structure for file releases to Affiliated Centres, suitable for a variety of computer installations.

New Search Strategies. The above integration means that bibliographic, connectivity and certain numeric items may now be searched together, rather than separately.To speed these searches a system of screens is being added to the file, based on numeric keys, hash-coding of text and bit screens for connectivity. Screenout rates of at least 96% have been achieved for a variety of bibliographic queries, leaving only 4% of entries for a full text match in the worst case. Ultimately the software will take advantage of chemical graphics to improve output. An enhanced system for query input is also planned.

19.2–1 COMPUTER ANIMATION AS AN AID TO CHEMICAL UNDERSTANDING

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Computer Graphics is slowly displacing static mechanical models in popularity as an aid to the better understanding of chemical structure. We had no display devices working fast enough to show realistic moving structures and reactions, so we decided to use computer animation on film.

The III FR80 microfilm recorder was used to make a 16mm colour film, 'Silicates in Solution', which shows some of the possible mechanisms involved when silicates encounter water molecules in solution. Our approach to the problems of production is discussed, some typical computing times given and some still sequences from the film displayed.

Existing computer programs were used as far as possible; most of the moving sequences were made using PLUTO78, but we found it necessary to write a new one, TETRA, to simplify the manipulation of the shaded tetrahedra shown in the latter part of the film.