Computer Program Abstracts

*The category Computer Program Abstracts provides a rapid means of communicating up-to-date information concerning both new programs or systems and significant updates to existing ones. Following normal submission, a Computer Program Abstract will be reviewed by one or two members of the IUCr Commission on Crystallographic Computing. It should not exceed 500 words in length and should use the standard format given on page 189 of the June 1985 issue of the Journal [J. Appl. Cryst. (1985), **18**, 189–190].*

J. Appl. Cryst. (1992). **25**, 663

CSDSHL – a utility for converting Cambridge Structual Database atom coordinate files to *SHELX* format.

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(*Received* 10 *December* 1991; *accepted* 24 *February* 1992)

The crystallographic problem: Graphically comparing published structures with structures recently determined involves not only composing the plot but also locating the published structure(s) and abstracting and formatting the atomic coordjnates into a style suitable for use in a graphics program. The *SHELXTL* graphics software has the capability of overlaying one structure on top of another. The Cambridge Structural Database System, CSD (Allen, Kennard & Taylor, 1983) provides a logical source of structural data for the published structures; however, this database system has no direct interface to program systems such as *SHELXTL* (Sheldrick, 1991). The *CSDSHL* routine provides a direct interface from the CSD to *SHELXTL*. This direct path can also be used to incorporate structural fragments into structure-solving programs such as *PATSEE* and *MULTAN*.

Method of solution: The structural results from a CSD search are first saved in an FDAT file. The program *CSDSHL*, which only requests the name of the FDAT file, is run. *CSDSHL* then creates ASCII file(s) named refcode.INS for each refcode containing coordinates in the FDAT file.

Software and hardware environments: The program was written in Fortran77 and has been implemented on a VAX station 4000 Model 300 running VMS 5.4-2, on a DEC Station 5000 Model 200 running ULTRIX version 4.1, on a SUN Sparcstation I running SUN OS 4.0.3, and on a Silicon Graphics Indigo running IRIX System V.3. A small modification for the UNIX systems is indicated in the source code.

Program specifications: Several points should be made about the output. Cell centering operations are explicitly translated to SYMM instructions rather than being incorporated into the LATT instruction of the output file. *SHELX* limits atom names to four characters, although CSD permits atom names of up to six characters. *CSDSHL* renames all atoms by appending a sequence number of the particular type of atom to the atomic symbol. Thus, the maximum number of atoms of a particular type with an atomic symbol of one character is 999 and the number of atoms with an atomic symbol of two characters is limited to 99. There is a current limit of 1000 atoms overall. This 1000-atom limit is easily changed in the source code with a PARAMETER instruction. The output files do not specify site occupancy factors or thermal parameters for the atoms. No constraints or restraints are placed upon the atom coordinates. The default radiation is Cu, since this information is not available in the FDAT file. A default UNIT instruction with one atom for each atom type is included in the output files.

Documentation and availability: Documentation is included in the source codes; source codes are available either by e-mail (preferred method) from powell@chem.wisc.edu or by floppy disk.

Keywords: Cambridge Structural Database (CSD), SHELX.

References

Allen, F. H., Kennard, O. & Taylor, R. (1983) *Acc. Chem. Res.* **16**, 146–153.

Sheldrick, G. M. (1991). *SHELXTL-Plus*. Version 4.2. Siemens Analytical Instruments, Madison, Wisconsin, USA.

Crystallographers

This section is intended to be a series of short paragraphs dealing with the activities of crystallographers, such as their changes of position, promotions, assumption of significant new duties, honours, etc. Items for inclusion, subject to the approval of the Editorial Board, should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England).

J. Appl. Cryst. (1992). **25**, 663

Professor **P. Berg,** Willson Professor of Biochemistry at Stanford University, USA, has been elected a Foreign Member of the Royal Society. He is distinguished for contributing the key discoveries which started genetic engineering. He was the first to construct a recombinant DNA molecule and, subsequently, took the lead in addressing the ethical considerations posed by DNA recombination research. He was awarded the Nobel Prize for Chemistry in 1980.

Mr **Dermott Wood,** recently retired from the BP Research Centre, Sunbury, England, is the first recipient of the Industrial Crystallography Award of the British Crystallographic Association. The award was instigated in 1991 as a means of being able to recognize sustained contributions to industrial crystallography by those who would find it difficult to be eligible for the more traditional awards that are made for outstanding contributions through publications *etc.* The presentation of the award was not viewed as a necessarily regular yearly event.

The award, in this case a Beevers model of montmorillonite, was made to Mr Wood during the Autumn Meeting of the Industrial Group on 7 November 1991. His work involved predominantly powder diffraction on a variety of different catalysts, minerals, deposits and corrosion products. He is probably best known for the methods that he developed for automated quantitative analysis of North Sea sandstones – up to 15 phases were identified and quantified.

Professor **W. P. Jencks,** Professor of Biochemistry at Brandeis University, USA, has been elected a Foreign Member of the Royal Society. He is distinguished for his outstanding work in the area of bio-organic mechanism, which revolutionized thinking at the molecular level of the extraordinary efficiency of enzyme catalysis.

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J. Appl. Cryst. (1992). **25**, 663–664

Refrigerated Air Stream for X-ray Diffraction

Mechanically refrigerated systems provide a constant flow of dry air or