

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 Structural Database atom coordinate files to SHELX format. By DOUGLAS R. POWELL, *Department of Chemistry, University of Wisconsin, Madison, WI 53706, USA*

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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 coordinates 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 *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).

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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 engi-

neering. 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.

New Commercial Products

Announcements of new commercial products are published by the *Journal of Applied Crystallography* free of charge. The descriptions, up to 300 words or the equivalent if a figure is included, should give the price and the manufacturer's full address. Full or partial inclusion is subject to the Editor's approval and to the space available. All correspondence should be sent to the Editor, Dr A. M. Glazer, Editor *Journal of Applied Crystallography*, Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, England.

The International Union of Crystallography can assume no responsibility for the accuracy of the claims made. A copy of the version sent to the printer is sent to the company concerned.

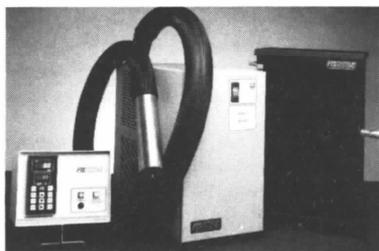
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Refrigerated Air Stream for X-ray Diffraction

Mechanically refrigerated systems provide a constant flow of dry air or

other gas, controllable from -85 to $+100^{\circ}\text{C}$ or -40 to $+100^{\circ}\text{C}$, for temperature control of X-ray diffraction samples with unattended operation. They eliminate the need to replace or refill liquid-nitrogen dewars in the middle of an experiment.

The **XR series of Air-Jet Crystal Coolers** have been used by many researchers, especially in protein crystal work. The gas-stream technique provides a desirable means to temperature control samples in a manner that does not interfere with visual observation or physical measurements. They are also used for temperature control in NMR studies.



FTS Systems Air-Jet Crystal Cooler

A new brochure describes the features, options, and operation of the system,

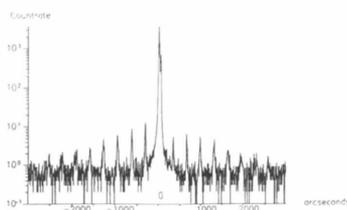
Joe Brendle, FTS Systems, Inc., PO Box 158, RT209, Stone Ridge, NY, USA 12484-0158.

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Enhanced Dynamic Range X-ray Detector from Bede Scientific

Bede Scientific have recently launched an **enhanced dynamic range (EDR) X-ray detector**, both as an integral feature of their high-resolution dif-

fraction and reflectivity systems and as a stand-alone product. The new device is a fast scintillation detector that gives a typical background count of 0.15 counts s^{-1} and peak count rates over $500\,000$ counts s^{-1} . Scintillation counters do not suffer the ageing effects inherent in proportional counters and by exploiting a recently developed photomultiplier tube, made from low-activity glass, with a linearly focused dynode array behind a 1 in aperture scintillation crystal, Bede Scientific have developed a system delivering a 5 V TTL output pulse of width 500 ns . The complete system consists of the detector head, including the pre-amplifier, together with a stand-alone electronics rack. This contains a high-stability EHT module, threshold and window discriminators and a digital ratemeter in addition to the TTL output.



Unsmoothed rocking curve of 50 period GaAlAs/GaAs MQW structure, $\text{Cu K}\alpha$ 002 reflection, with 10 s count time per point

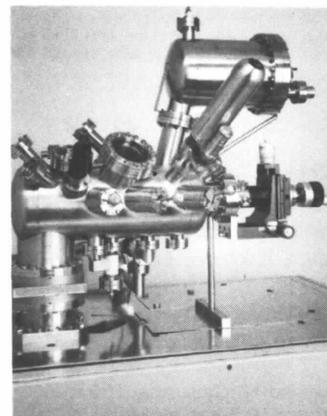
Bede Scientific, Lindsey Park, Bowburn, Durham DH6 5PF, England.

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Combined STM/XPS Instrument Delivered to Japan

A major combined **STM/XPS system**, supplied by VG Microtech, has recently

been accepted by the user in Japan. The instrument will be used to study thin metal films deposited in an adjoining UHV system – the user is working to integrate the two systems over the next few months. The system is capable of atomic resolution imaging in the STM and high-performance XPS.



Combined UHV STM/XPS instrument from VG Microtech

The major components of the instrument are a VG STM2000 scanning tunnelling microscope, CLAM2 analyser, X-ray source and five-axis sample manipulator. During XPS analysis the specimen is mounted on the manipulator and can then be transferred by means of pincer-grip wobblesticks to the STM.

The instrument can be upgraded with additional analytical techniques, such as Auger electron spectroscopy, by fitting electron guns, ion guns, gas leak valves, etc.

VG Microtech, Bellbrook Business Park, Bell Lane, Uckfield, East Sussex TN22 1QZ, England.